



Full wwPDB NMR Structure Validation Report ⓘ

Oct 11, 2021 – 08:19 AM EDT

PDB ID : 2K01
Title : Structure of a locked SDF1 dimer
Authors : Volkman, B.F.; Veldkamp, C.T.; Peterson, F.C.
Deposited on : 2008-01-23

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.23.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

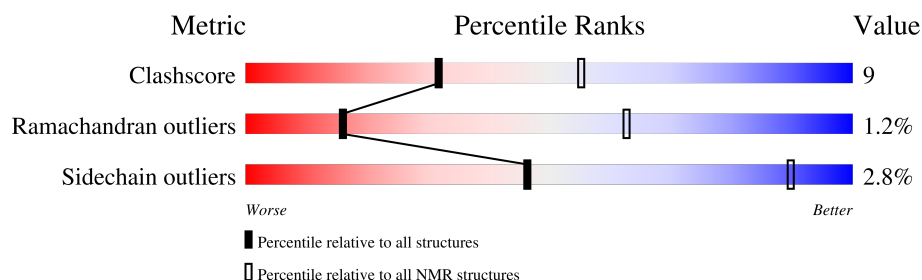
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 84%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	70	
1	C	70	

2 Ensemble composition and analysis

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:11-A:43, A:47-A:67, C:211-C:243, C:247-C:268 (109)	0.38	5

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 5 clusters and 5 single-model clusters were found.

Cluster number	Models
1	1, 9, 13, 14
2	5, 11, 16, 19
3	3, 4, 7
4	10, 15
5	18, 20
Single-model clusters	2; 6; 8; 12; 17

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2273 atoms, of which 1158 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Stromal cell-derived factor 1.

Mol	Chain	Residues	Atoms						Trace
1	A	68	Total	C	H	N	O	S	0
			1136	353	579	106	92	6	
1	C	68	Total	C	H	N	O	S	0
			1137	353	579	106	93	6	

There are 8 discrepancies between the modelled and reference sequences:

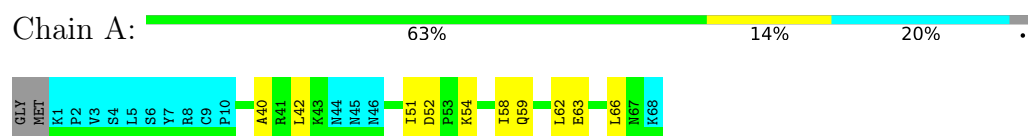
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P48061
A	0	MET	-	expression tag	UNP P48061
A	36	CYS	LEU	engineered mutation	UNP P48061
A	65	CYS	ALA	engineered mutation	UNP P48061
C	199	GLY	-	expression tag	UNP P48061
C	200	MET	-	expression tag	UNP P48061
C	236	CYS	LEU	engineered mutation	UNP P48061
C	265	CYS	ALA	engineered mutation	UNP P48061

4 Residue-property plots [i](#)

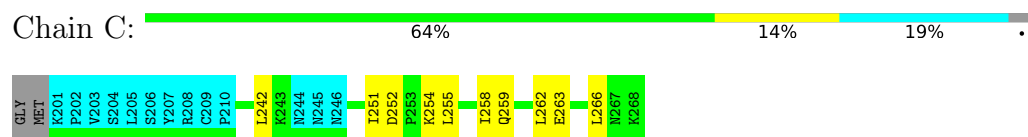
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Stromal cell-derived factor 1



- Molecule 1: Stromal cell-derived factor 1

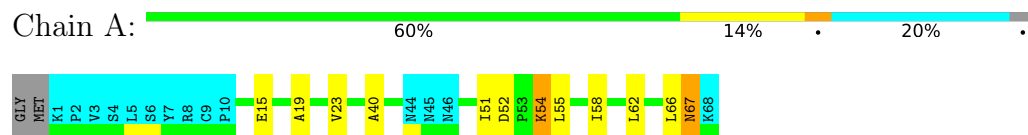


4.2 Scores per residue for each member of the ensemble

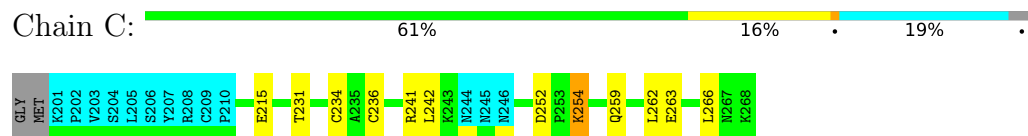
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Stromal cell-derived factor 1

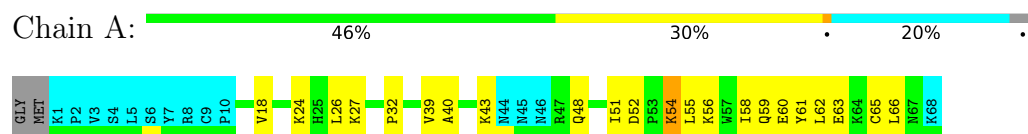


- Molecule 1: Stromal cell-derived factor 1

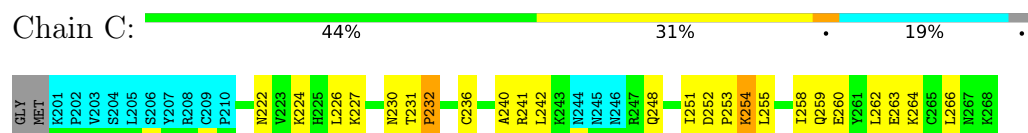


4.2.2 Score per residue for model 2

- Molecule 1: Stromal cell-derived factor 1

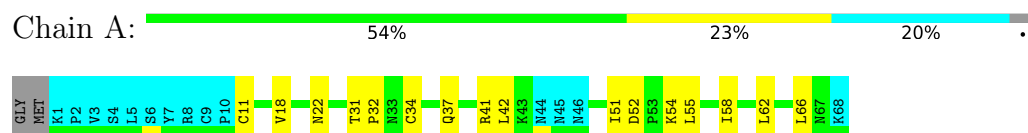


- Molecule 1: Stromal cell-derived factor 1

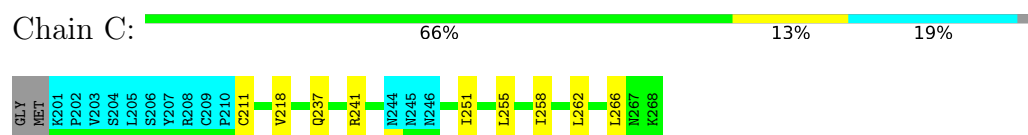


4.2.3 Score per residue for model 3

- Molecule 1: Stromal cell-derived factor 1

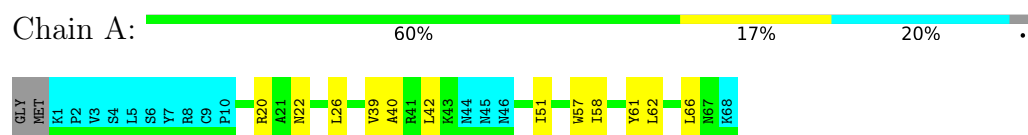


- Molecule 1: Stromal cell-derived factor 1

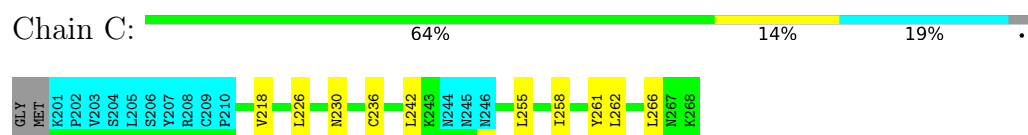


4.2.4 Score per residue for model 4

- Molecule 1: Stromal cell-derived factor 1

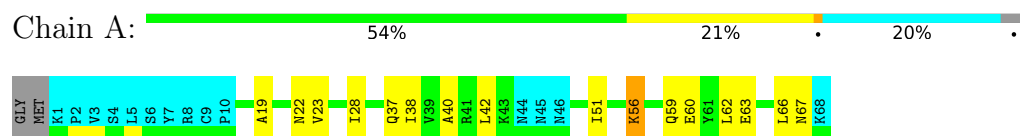


- Molecule 1: Stromal cell-derived factor 1

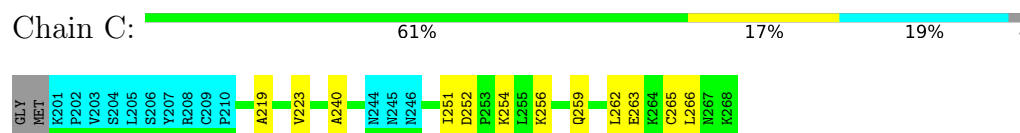


4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Stromal cell-derived factor 1

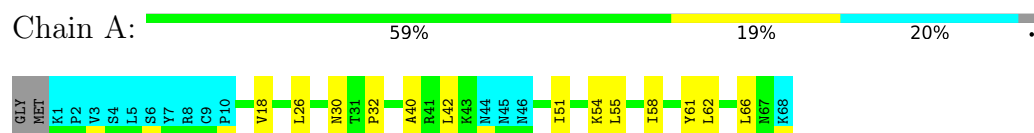


- Molecule 1: Stromal cell-derived factor 1



4.2.6 Score per residue for model 6

- Molecule 1: Stromal cell-derived factor 1

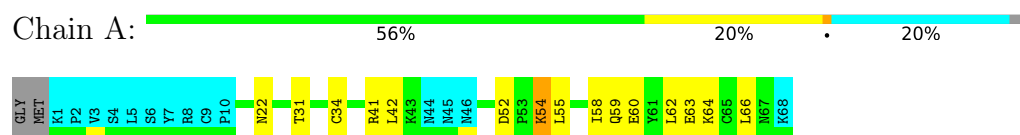


- Molecule 1: Stromal cell-derived factor 1

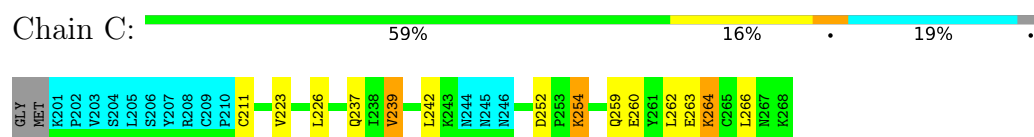


4.2.7 Score per residue for model 7

- Molecule 1: Stromal cell-derived factor 1

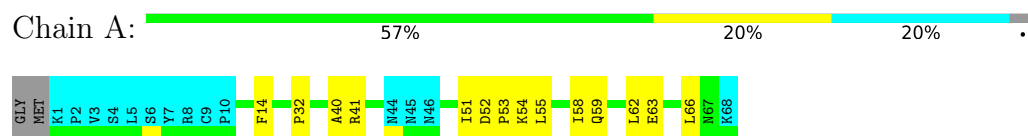


- Molecule 1: Stromal cell-derived factor 1



4.2.8 Score per residue for model 8

- Molecule 1: Stromal cell-derived factor 1

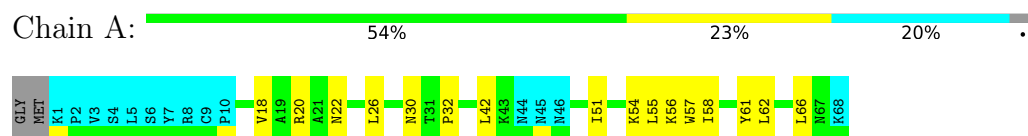


- Molecule 1: Stromal cell-derived factor 1

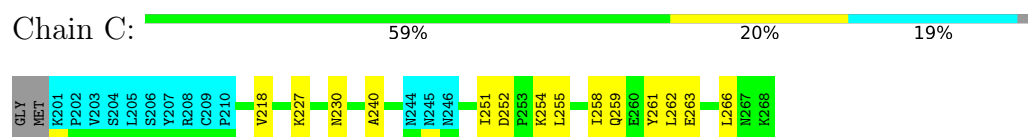


4.2.9 Score per residue for model 9

- Molecule 1: Stromal cell-derived factor 1

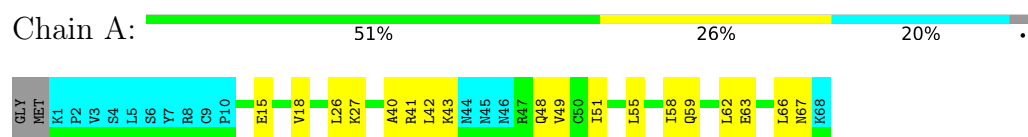


- Molecule 1: Stromal cell-derived factor 1

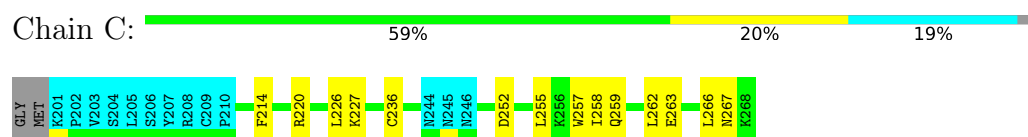


4.2.10 Score per residue for model 10

- Molecule 1: Stromal cell-derived factor 1

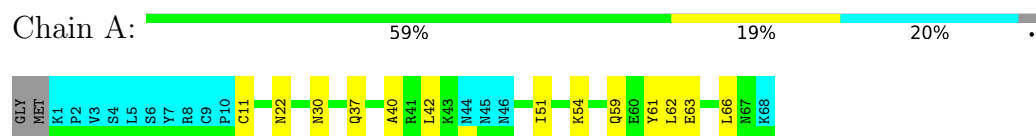


- Molecule 1: Stromal cell-derived factor 1

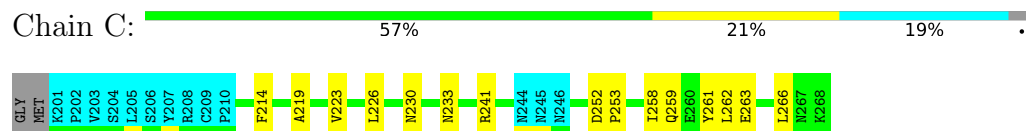


4.2.11 Score per residue for model 11

- Molecule 1: Stromal cell-derived factor 1

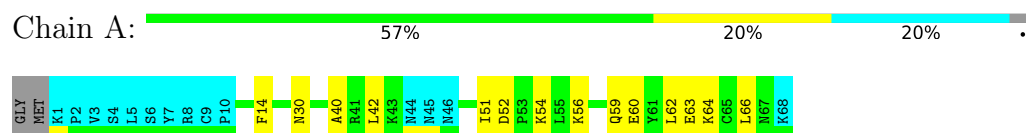


- Molecule 1: Stromal cell-derived factor 1

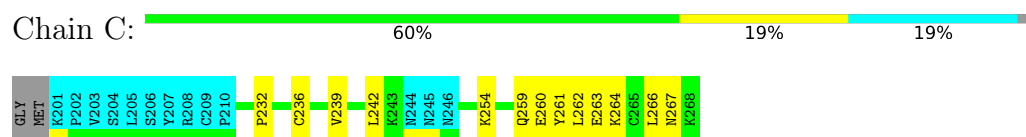


4.2.12 Score per residue for model 12

- Molecule 1: Stromal cell-derived factor 1

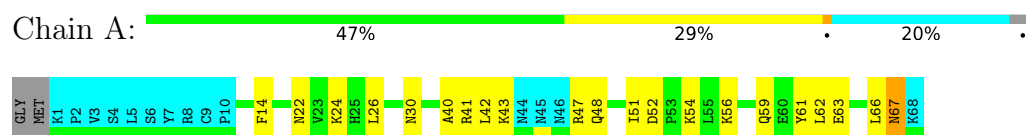


- Molecule 1: Stromal cell-derived factor 1

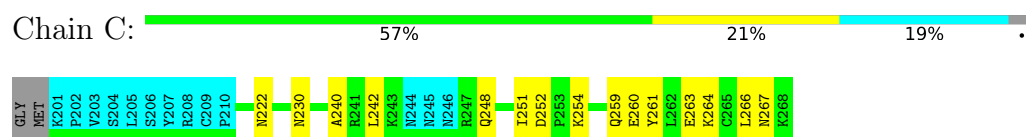


4.2.13 Score per residue for model 13

- Molecule 1: Stromal cell-derived factor 1

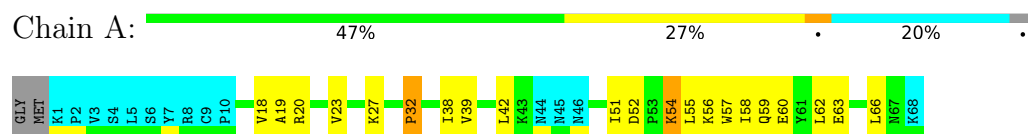


- Molecule 1: Stromal cell-derived factor 1

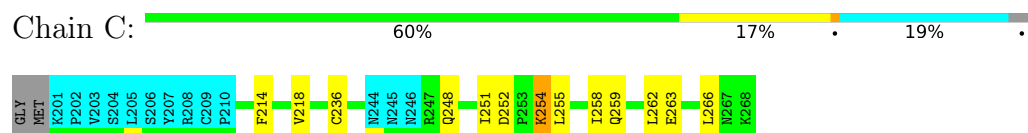


4.2.14 Score per residue for model 14

- Molecule 1: Stromal cell-derived factor 1

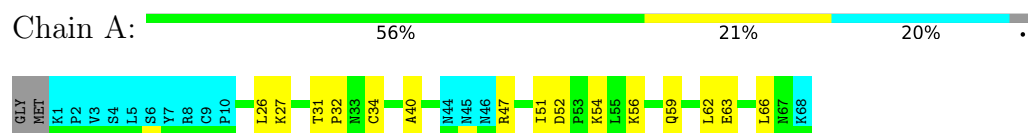


- Molecule 1: Stromal cell-derived factor 1

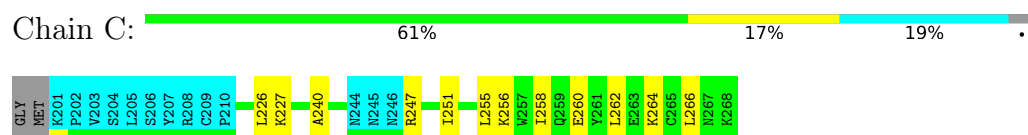


4.2.15 Score per residue for model 15

- Molecule 1: Stromal cell-derived factor 1

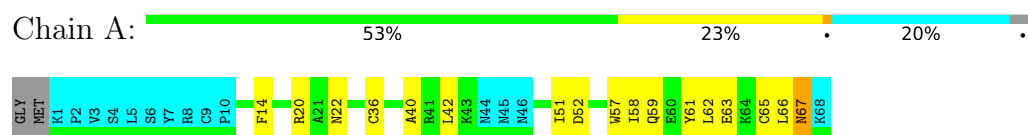


- Molecule 1: Stromal cell-derived factor 1

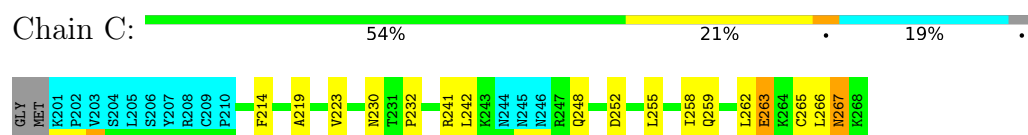


4.2.16 Score per residue for model 16

- Molecule 1: Stromal cell-derived factor 1

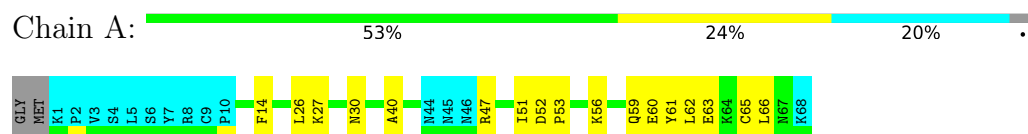


- Molecule 1: Stromal cell-derived factor 1

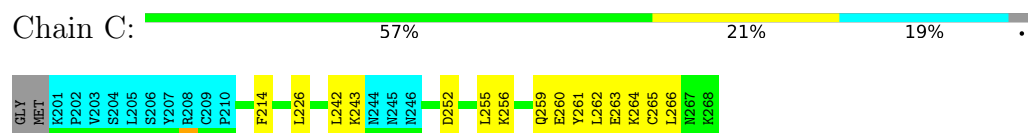


4.2.17 Score per residue for model 17

- Molecule 1: Stromal cell-derived factor 1

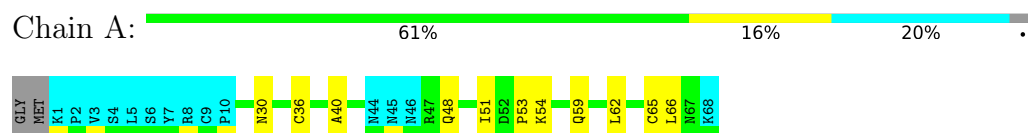


- Molecule 1: Stromal cell-derived factor 1

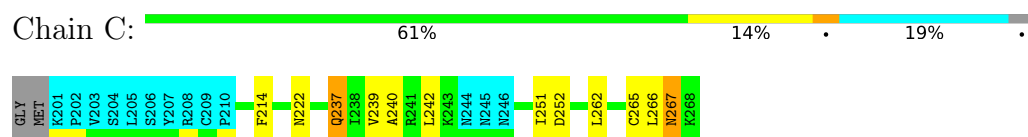


4.2.18 Score per residue for model 18

- Molecule 1: Stromal cell-derived factor 1

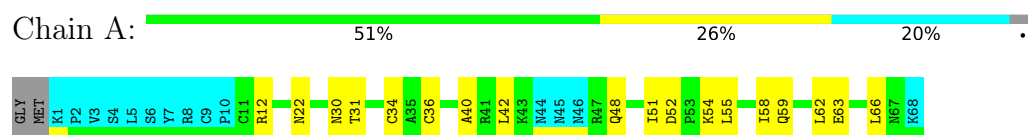


- Molecule 1: Stromal cell-derived factor 1

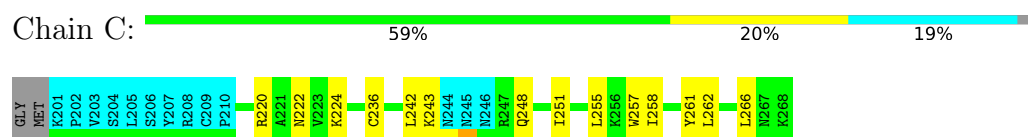


4.2.19 Score per residue for model 19

- Molecule 1: Stromal cell-derived factor 1



- Molecule 1: Stromal cell-derived factor 1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *AUTOMATED METHODS WERE USED FOR BACKBONE CHEMICAL SHIFT ASSIGNMENT AND ITERATIVE NOE REFINEMENT. FINAL STRUCTURES WERE OBTAINED BY MOLECULAR DYNAMICS IN EXPLICIT SOLVENT, AUTOMATED METHODS WERE USED FOR BACKBONE CHEMICAL SHIFT ASSIGNMENT AND ITERATIVE NOE REFINEMENT. FINAL STRUCTURES WERE OBTAINED BY MOLECULAR DYNAMICS IN EXPLICIT SOLVENT.*

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
Xplor-NIH	refinement	2.9.3

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	3238
Number of shifts mapped to atoms	1622
Number of unparsed shifts	1616
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	445	465	463	11±3
1	C	455	478	476	10±3
All	All	18000	18860	18780	349

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:GLN:O	1:A:63:GLU:HB2	0.68	1.88	20	6
1:A:62:LEU:HD11	1:C:266:LEU:HD21	0.66	1.68	10	19
1:C:259:GLN:O	1:C:263:GLU:HB2	0.65	1.92	20	8
1:A:59:GLN:OE1	1:C:266:LEU:HA	0.62	1.94	12	1
1:A:52:ASP:OD1	1:A:54:LYS:HG2	0.62	1.95	7	7
1:C:252:ASP:OD1	1:C:254:LYS:HG2	0.61	1.96	2	5
1:A:63:GLU:HA	1:A:66:LEU:HD12	0.61	1.72	12	4
1:A:30:ASN:HB2	1:C:261:TYR:OH	0.60	1.97	13	6
1:A:61:TYR:OH	1:C:230:ASN:HB2	0.59	1.98	13	6
1:A:66:LEU:HA	1:C:259:GLN:OE1	0.58	1.97	7	2
1:A:52:ASP:OD2	1:A:54:LYS:HG2	0.58	1.99	13	1
1:C:263:GLU:HA	1:C:266:LEU:HD12	0.57	1.76	10	8
1:A:22:ASN:OD1	1:A:42:LEU:HB3	0.55	2.00	4	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:LEU:HD21	1:C:262:LEU:HD11	0.55	1.77	19	19
1:C:218:VAL:HG21	1:C:251:ILE:CG2	0.54	2.33	14	5
1:C:259:GLN:O	1:C:263:GLU:HG3	0.54	2.03	6	6
1:A:67:ASN:H	1:C:259:GLN:NE2	0.54	2.01	10	2
1:A:30:ASN:HA	1:C:261:TYR:OH	0.54	2.03	17	1
1:C:231:THR:OG1	1:C:234:CYS:HB2	0.53	2.04	20	2
1:C:255:LEU:O	1:C:258:ILE:HB	0.52	2.04	4	12
1:C:222:ASN:OD1	1:C:242:LEU:HB3	0.51	2.05	20	3
1:C:214:PHE:CG	1:C:252:ASP:HB2	0.51	2.40	11	8
1:A:62:LEU:HA	1:A:65:CYS:SG	0.51	2.44	17	3
1:A:59:GLN:O	1:A:63:GLU:HG3	0.51	2.04	8	7
1:A:51:ILE:CD1	1:A:58:ILE:HD11	0.51	2.36	2	5
1:C:260:GLU:O	1:C:264:LYS:HG2	0.51	2.06	2	7
1:A:20:ARG:HB2	1:A:57:TRP:CE3	0.50	2.42	14	4
1:A:59:GLN:OE1	1:C:266:LEU:HD23	0.50	2.05	12	1
1:A:55:LEU:O	1:A:58:ILE:HB	0.50	2.07	2	10
1:A:62:LEU:HD11	1:C:266:LEU:CD2	0.49	2.37	8	5
1:C:262:LEU:HA	1:C:265:CYS:SG	0.49	2.48	18	2
1:A:40:ALA:HB2	1:A:51:ILE:HD13	0.49	1.83	15	16
1:C:254:LYS:HA	1:C:254:LYS:HE2	0.49	1.85	9	1
1:C:254:LYS:HE2	1:C:254:LYS:HA	0.49	1.84	6	4
1:C:231:THR:HB	1:C:234:CYS:O	0.48	2.07	6	1
1:A:66:LEU:CD2	1:C:262:LEU:HD11	0.48	2.38	11	5
1:C:264:LYS:HE3	1:C:264:LYS:HA	0.48	1.85	20	2
1:A:66:LEU:HD11	1:C:266:LEU:HD11	0.48	1.84	11	1
1:A:31:THR:HB	1:A:34:CYS:O	0.48	2.07	15	1
1:C:252:ASP:OD2	1:C:254:LYS:HB2	0.48	2.09	5	1
1:A:54:LYS:HA	1:A:59:GLN:NE2	0.48	2.23	11	3
1:A:18:VAL:HG21	1:A:51:ILE:CG2	0.48	2.38	14	4
1:A:60:GLU:O	1:A:64:LYS:HG2	0.48	2.09	20	3
1:A:66:LEU:HD23	1:C:259:GLN:OE1	0.48	2.08	7	2
1:A:54:LYS:HA	1:A:54:LYS:HE2	0.48	1.85	9	5
1:A:67:ASN:N	1:A:67:ASN:HD22	0.47	2.07	16	1
1:C:256:LYS:O	1:C:260:GLU:HG3	0.47	2.09	17	2
1:A:14:PHE:CG	1:A:52:ASP:HB2	0.47	2.44	16	6
1:A:59:GLN:NE2	1:C:267:ASN:H	0.47	2.08	18	3
1:A:67:ASN:HD22	1:A:67:ASN:N	0.47	2.08	13	2
1:A:27:LYS:HA	1:C:226:LEU:O	0.47	2.10	10	4
1:A:54:LYS:HE3	1:A:54:LYS:HA	0.47	1.86	7	2
1:A:56:LYS:O	1:A:60:GLU:HG3	0.46	2.09	12	5
1:A:31:THR:OG1	1:A:34:CYS:HB2	0.46	2.11	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:226:LEU:HD12	1:C:261:TYR:CD2	0.46	2.45	4	2
1:C:218:VAL:HG23	1:C:242:LEU:HD21	0.46	1.86	4	2
1:A:52:ASP:OD2	1:A:54:LYS:HB2	0.46	2.11	15	2
1:A:26:LEU:O	1:C:227:LYS:HA	0.45	2.11	15	4
1:A:59:GLN:HE22	1:C:267:ASN:H	0.45	1.54	10	2
1:C:211:CYS:HB2	1:C:237:GLN:NE2	0.45	2.26	3	2
1:A:26:LEU:HD12	1:A:61:TYR:CD2	0.45	2.47	17	2
1:C:242:LEU:HD22	1:C:242:LEU:N	0.45	2.27	17	1
1:C:219:ALA:O	1:C:223:VAL:HG23	0.45	2.12	16	3
1:C:267:ASN:HD22	1:C:267:ASN:N	0.45	2.10	16	1
1:A:18:VAL:HG23	1:A:42:LEU:HD21	0.45	1.89	6	1
1:C:251:ILE:CD1	1:C:258:ILE:HD11	0.45	2.42	19	3
1:C:226:LEU:HA	1:C:239:VAL:O	0.44	2.12	7	1
1:A:27:LYS:O	1:A:38:ILE:HA	0.44	2.13	14	1
1:C:254:LYS:HE3	1:C:254:LYS:HA	0.44	1.87	14	1
1:A:19:ALA:O	1:A:23:VAL:HG23	0.44	2.13	5	3
1:C:220:ARG:HB2	1:C:257:TRP:CE3	0.44	2.48	10	4
1:A:18:VAL:HG13	1:A:42:LEU:HD21	0.44	1.88	9	1
1:A:11:CYS:HB2	1:A:37:GLN:NE2	0.44	2.28	11	2
1:C:240:ALA:HB2	1:C:251:ILE:HD13	0.43	1.88	5	7
1:A:28:ILE:HA	1:A:37:GLN:O	0.43	2.14	5	1
1:C:222:ASN:ND2	1:C:242:LEU:HD13	0.43	2.29	8	3
1:A:54:LYS:HA	1:A:54:LYS:CE	0.43	2.44	6	2
1:C:223:VAL:HG22	1:C:242:LEU:CD2	0.43	2.44	7	2
1:C:226:LEU:HD12	1:C:261:TYR:CD1	0.43	2.48	11	1
1:A:65:CYS:HB3	1:C:253:PRO:HB3	0.43	1.90	2	1
1:A:24:LYS:HD3	1:A:41:ARG:HD2	0.43	1.90	13	1
1:A:15:GLU:HG3	1:A:49:VAL:HB	0.43	1.91	10	1
1:A:38:ILE:HD11	1:C:265:CYS:SG	0.43	2.54	5	1
1:A:53:PRO:CB	1:C:265:CYS:HB3	0.42	2.44	17	1
1:A:42:LEU:N	1:A:42:LEU:HD22	0.42	2.29	10	1
1:C:252:ASP:O	1:C:255:LEU:HG	0.42	2.14	17	1
1:C:222:ASN:O	1:C:243:LYS:HG2	0.42	2.15	19	1
1:C:237:GLN:HE21	1:C:237:GLN:HA	0.42	1.74	18	1
1:A:53:PRO:HB3	1:C:265:CYS:HB3	0.42	1.91	20	2
1:A:12:ARG:HD3	1:A:12:ARG:O	0.41	2.15	19	1
1:C:224:LYS:CG	1:C:243:LYS:HB3	0.41	2.45	19	1
1:A:36:CYS:O	1:A:53:PRO:HG3	0.41	2.16	18	1
1:A:51:ILE:HD11	1:A:58:ILE:HD11	0.41	1.92	2	1
1:A:40:ALA:HB2	1:A:51:ILE:CD1	0.41	2.46	4	2
1:A:53:PRO:HA	1:A:58:ILE:HG21	0.41	1.91	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:LEU:HD12	1:A:61:TYR:CD1	0.41	2.51	13	1
1:C:254:LYS:HA	1:C:254:LYS:CE	0.41	2.45	12	1
1:A:59:GLN:O	1:A:63:GLU:HG2	0.41	2.15	15	1
1:A:31:THR:HG21	1:A:34:CYS:HB2	0.41	1.91	3	1
1:C:259:GLN:O	1:C:263:GLU:HG2	0.41	2.15	5	1
1:A:24:LYS:HG2	1:A:43:LYS:HB3	0.41	1.92	2	1
1:C:268:LYS:NZ	1:C:268:LYS:HB3	0.41	2.31	6	1
1:A:18:VAL:HG23	1:A:42:LEU:HD11	0.41	1.93	10	1
1:C:242:LEU:N	1:C:242:LEU:HD22	0.40	2.31	12	1
1:A:62:LEU:HB2	1:C:262:LEU:HB2	0.40	1.94	15	1
1:A:64:LYS:HA	1:A:64:LYS:HE2	0.40	1.92	20	1
1:C:252:ASP:OD2	1:C:254:LYS:HG2	0.40	2.17	13	1
1:A:26:LEU:HA	1:A:39:VAL:O	0.40	2.17	4	2
1:C:253:PRO:HA	1:C:258:ILE:HG21	0.40	1.93	11	1
1:A:42:LEU:HD22	1:A:42:LEU:N	0.40	2.31	13	1
1:C:224:LYS:HD3	1:C:241:ARG:HG3	0.40	1.92	2	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	54/70 (77%)	50±1 (93±2%)	3±1 (6±2%)	1±1 (1±1%)	20	68
1	C	54/70 (77%)	50±1 (92±2%)	4±1 (7±2%)	1±1 (1±1%)	14	59
All	All	2160/2800 (77%)	1994 (92%)	139 (6%)	27 (1%)	16	63

All 9 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	C	236	CYS	7
1	A	32	PRO	5
1	C	232	PRO	3
1	C	267	ASN	3
1	A	47	ARG	3

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Mol	Chain	Res	Type	Models (Total)
1	A	36	CYS	3
1	C	217	HIS	1
1	C	247	ARG	1
1	C	243	LYS	1

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	50/65 (77%)	49±1 (97±2%)	1±1 (3±2%)	46	90
1	C	51/65 (78%)	50±1 (97±2%)	1±1 (3±2%)	46	90
All	All	2020/2600 (78%)	1963 (97%)	57 (3%)	46	90

All 21 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	C	248	GLN	6
1	A	48	GLN	5
1	A	56	LYS	5
1	A	54	LYS	4
1	C	241	ARG	4
1	C	254	LYS	4
1	A	41	ARG	4
1	C	239	VAL	4
1	A	67	ASN	3
1	C	267	ASN	3
1	C	256	LYS	2
1	C	264	LYS	2
1	A	43	LYS	2
1	A	39	VAL	2
1	A	15	GLU	1
1	C	215	GLU	1
1	C	268	LYS	1
1	A	42	LEU	1
1	C	263	GLU	1
1	A	47	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	C	237	GLN	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 84% for the well-defined parts and 80% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	3238
Number of shifts mapped to atoms	1622
Number of unparsed shifts	1616
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. All 1616 occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1623	A	1	LYS	H	8.483	0.020	1
1624	C	201	LYS	H	8.483	0.020	1
1625	A	1	LYS	N	124.855	0.1	1
1626	C	201	LYS	N	124.855	0.1	1
1627	A	2	PRO	HA	4.490	0.020	1
1628	C	202	PRO	HA	4.490	0.020	1
1629	A	2	PRO	HB2	2.329	0.005	2
1630	C	202	PRO	HB2	2.329	0.005	2
1631	A	2	PRO	HB3	1.931	0.008	2
1632	C	202	PRO	HB3	1.931	0.008	2
1633	A	2	PRO	HD2	3.883	0.004	2
1634	C	202	PRO	HD2	3.883	0.004	2
1635	A	2	PRO	HD3	3.668	0.020	2
1636	C	202	PRO	HD3	3.668	0.020	2
1637	A	2	PRO	HG2	2.068	0.008	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1638	C	202	PRO	HG2	2.068	0.008	2
1639	A	2	PRO	HG3	2.068	0.008	2
1640	C	202	PRO	HG3	2.068	0.008	2
1641	A	2	PRO	C	177.102	0.1	1
1642	C	202	PRO	C	177.102	0.1	1
1643	A	2	PRO	CA	63.319	0.1	1
1644	C	202	PRO	CA	63.319	0.1	1
1645	A	2	PRO	CB	32.575	0.1	1
1646	C	202	PRO	CB	32.575	0.1	1
1647	A	2	PRO	CD	51.111	0.044	1
1648	C	202	PRO	CD	51.111	0.044	1
1649	A	2	PRO	CG	27.806	0.101	1
1650	C	202	PRO	CG	27.806	0.101	1
1651	A	3	VAL	H	8.259	0.020	1
1652	C	203	VAL	H	8.259	0.020	1
1653	A	3	VAL	HA	4.117	0.020	1
1654	C	203	VAL	HA	4.117	0.020	1
1655	A	3	VAL	HB	2.087	0.020	1
1656	C	203	VAL	HB	2.087	0.020	1
1657	A	3	VAL	HG11	0.977	0.020	2
1658	C	203	VAL	HG11	0.977	0.020	2
1659	A	3	VAL	HG12	0.977	0.020	2
1660	C	203	VAL	HG12	0.977	0.020	2
1661	A	3	VAL	HG13	0.977	0.020	2
1662	C	203	VAL	HG13	0.977	0.020	2
1663	A	3	VAL	HG21	0.977	0.020	2
1664	C	203	VAL	HG21	0.977	0.020	2
1665	A	3	VAL	HG22	0.977	0.020	2
1666	C	203	VAL	HG22	0.977	0.020	2
1667	A	3	VAL	HG23	0.977	0.020	2
1668	C	203	VAL	HG23	0.977	0.020	2
1669	A	3	VAL	C	176.385	0.1	1
1670	C	203	VAL	C	176.385	0.1	1
1671	A	3	VAL	CA	62.629	0.1	1
1672	C	203	VAL	CA	62.629	0.1	1
1673	A	3	VAL	CB	33.146	0.1	1
1674	C	203	VAL	CB	33.146	0.1	1
1675	A	3	VAL	CG1	21.102	0.057	1
1676	C	203	VAL	CG1	21.102	0.057	1
1677	A	3	VAL	CG2	21.159	0.1	1
1678	C	203	VAL	CG2	21.159	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1679	A	3	VAL	N	120.806	0.1	1
1680	C	203	VAL	N	120.806	0.1	1
1681	A	4	SER	H	8.345	0.020	1
1682	C	204	SER	H	8.345	0.020	1
1683	A	4	SER	HA	4.479	0.020	1
1684	C	204	SER	HA	4.479	0.020	1
1685	A	4	SER	HB2	3.864	0.020	2
1686	C	204	SER	HB2	3.864	0.020	2
1687	A	4	SER	HB3	3.864	0.020	2
1688	C	204	SER	HB3	3.864	0.020	2
1689	A	4	SER	C	174.687	0.1	1
1690	C	204	SER	C	174.687	0.1	1
1691	A	4	SER	CA	58.340	0.1	1
1692	C	204	SER	CA	58.340	0.1	1
1693	A	4	SER	CB	64.208	0.1	1
1694	C	204	SER	CB	64.208	0.1	1
1695	A	4	SER	N	119.332	0.1	1
1696	C	204	SER	N	119.332	0.1	1
1697	A	5	LEU	H	8.334	0.020	1
1698	C	205	LEU	H	8.334	0.020	1
1699	A	5	LEU	HA	4.384	0.020	1
1700	C	205	LEU	HA	4.384	0.020	1
1701	A	5	LEU	HB2	1.637	0.020	2
1702	C	205	LEU	HB2	1.637	0.020	2
1703	A	5	LEU	HB3	1.550	0.020	2
1704	C	205	LEU	HB3	1.550	0.020	2
1705	A	5	LEU	HD11	0.938	0.020	2
1706	C	205	LEU	HD11	0.938	0.020	2
1707	A	5	LEU	HD12	0.938	0.020	2
1708	C	205	LEU	HD12	0.938	0.020	2
1709	A	5	LEU	HD13	0.938	0.020	2
1710	C	205	LEU	HD13	0.938	0.020	2
1711	A	5	LEU	C	177.424	0.1	1
1712	C	205	LEU	C	177.424	0.1	1
1713	A	5	LEU	CA	55.495	0.1	1
1714	C	205	LEU	CA	55.495	0.1	1
1715	A	5	LEU	CB	42.786	0.1	1
1716	C	205	LEU	CB	42.786	0.1	1
1717	A	5	LEU	CD1	25.338	0.1	1
1718	C	205	LEU	CD1	25.338	0.1	1
1719	A	5	LEU	N	124.942	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1720	C	205	LEU	N	124.942	0.1	1
1721	A	6	SER	H	8.198	0.020	1
1722	C	206	SER	H	8.198	0.020	1
1723	A	6	SER	HA	4.407	0.020	1
1724	C	206	SER	HA	4.407	0.020	1
1725	A	6	SER	HB2	3.814	0.020	2
1726	C	206	SER	HB2	3.814	0.020	2
1727	A	6	SER	HB3	3.814	0.020	2
1728	C	206	SER	HB3	3.814	0.020	2
1729	A	6	SER	C	174.306	0.1	1
1730	C	206	SER	C	174.306	0.1	1
1731	A	6	SER	CA	58.696	0.1	1
1732	C	206	SER	CA	58.696	0.1	1
1733	A	6	SER	CB	64.136	0.1	1
1734	C	206	SER	CB	64.136	0.1	1
1735	A	6	SER	N	116.070	0.1	1
1736	C	206	SER	N	116.070	0.1	1
1737	A	7	TYR	H	8.005	0.020	1
1738	C	207	TYR	H	8.005	0.020	1
1739	A	7	TYR	HA	4.547	0.020	1
1740	C	207	TYR	HA	4.547	0.020	1
1741	A	7	TYR	HB2	3.069	0.020	2
1742	C	207	TYR	HB2	3.069	0.020	2
1743	A	7	TYR	HB3	2.952	0.020	2
1744	C	207	TYR	HB3	2.952	0.020	2
1745	A	7	TYR	HD1	7.124	0.020	1
1746	C	207	TYR	HD1	7.124	0.020	1
1747	A	7	TYR	HD2	7.124	0.020	1
1748	C	207	TYR	HD2	7.124	0.020	1
1749	A	7	TYR	HE1	6.861	0.002	1
1750	C	207	TYR	HE1	6.861	0.002	1
1751	A	7	TYR	HE2	6.861	0.002	1
1752	C	207	TYR	HE2	6.861	0.002	1
1753	A	7	TYR	C	175.507	0.1	1
1754	C	207	TYR	C	175.507	0.1	1
1755	A	7	TYR	CA	58.236	0.1	1
1756	C	207	TYR	CA	58.236	0.1	1
1757	A	7	TYR	CB	39.144	0.1	1
1758	C	207	TYR	CB	39.144	0.1	1
1759	A	7	TYR	CD1	133.342	0.1	1
1760	C	207	TYR	CD1	133.342	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1761	A	7	TYR	CE1	118.329	0.1	1
1762	C	207	TYR	CE1	118.329	0.1	1
1763	A	7	TYR	N	122.102	0.1	1
1764	C	207	TYR	N	122.102	0.1	1
1765	A	8	ARG	H	8.142	0.020	1
1766	C	208	ARG	H	8.142	0.020	1
1767	A	8	ARG	HA	4.302	0.010	1
1768	C	208	ARG	HA	4.302	0.010	1
1769	A	8	ARG	HB2	1.810	0.020	2
1770	C	208	ARG	HB2	1.810	0.020	2
1771	A	8	ARG	HB3	1.710	0.020	2
1772	C	208	ARG	HB3	1.710	0.020	2
1773	A	8	ARG	HD2	3.177	0.003	2
1774	C	208	ARG	HD2	3.177	0.003	2
1775	A	8	ARG	HD3	3.177	0.003	2
1776	C	208	ARG	HD3	3.177	0.003	2
1777	A	8	ARG	HG2	1.550	0.007	2
1778	C	208	ARG	HG2	1.550	0.007	2
1779	A	8	ARG	HG3	1.550	0.007	2
1780	C	208	ARG	HG3	1.550	0.007	2
1781	A	8	ARG	C	175.946	0.1	1
1782	C	208	ARG	C	175.946	0.1	1
1783	A	8	ARG	CA	56.102	0.1	1
1784	C	208	ARG	CA	56.102	0.1	1
1785	A	8	ARG	CB	31.004	0.1	1
1786	C	208	ARG	CB	31.004	0.1	1
1787	A	8	ARG	CD	43.900	0.1	1
1788	C	208	ARG	CD	43.900	0.1	1
1789	A	8	ARG	CG	26.854	0.1	1
1790	C	208	ARG	CG	26.854	0.1	1
1791	A	8	ARG	N	122.105	0.1	1
1792	C	208	ARG	N	122.105	0.1	1
1793	A	9	CYS	H	8.185	0.020	1
1794	C	209	CYS	H	8.185	0.020	1
1795	A	9	CYS	HA	4.952	0.006	1
1796	C	209	CYS	HA	4.952	0.006	1
1797	A	9	CYS	HB2	2.727	0.002	2
1798	C	209	CYS	HB2	2.727	0.002	2
1799	A	9	CYS	HB3	3.164	0.009	2
1800	C	209	CYS	HB3	3.164	0.009	2
1801	A	9	CYS	CA	53.192	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1802	C	209	CYS	CA	53.192	0.1	1
1803	A	9	CYS	CB	40.250	0.1	1
1804	C	209	CYS	CB	40.250	0.1	1
1805	A	9	CYS	N	121.511	0.1	1
1806	C	209	CYS	N	121.511	0.1	1
1807	A	10	PRO	HA	4.315	0.011	1
1808	C	210	PRO	HA	4.315	0.011	1
1809	A	10	PRO	HB2	1.915	0.006	2
1810	C	210	PRO	HB2	1.915	0.006	2
1811	A	10	PRO	HB3	2.364	0.005	2
1812	C	210	PRO	HB3	2.364	0.005	2
1813	A	10	PRO	HD2	3.891	0.006	2
1814	C	210	PRO	HD2	3.891	0.006	2
1815	A	10	PRO	HD3	3.891	0.006	2
1816	C	210	PRO	HD3	3.891	0.006	2
1817	A	10	PRO	HG2	2.102	0.007	2
1818	C	210	PRO	HG2	2.102	0.007	2
1819	A	10	PRO	HG3	2.102	0.007	2
1820	C	210	PRO	HG3	2.102	0.007	2
1821	A	10	PRO	C	177.980	0.1	1
1822	C	210	PRO	C	177.980	0.1	1
1823	A	10	PRO	CA	65.345	0.140	1
1824	C	210	PRO	CA	65.345	0.140	1
1825	A	10	PRO	CB	32.575	0.1	1
1826	C	210	PRO	CB	32.575	0.1	1
1827	A	10	PRO	CD	51.225	0.057	1
1828	C	210	PRO	CD	51.225	0.057	1
1829	A	10	PRO	CG	27.841	0.070	1
1830	C	210	PRO	CG	27.841	0.070	1
1831	A	11	CYS	H	8.719	0.020	1
1832	C	211	CYS	H	8.719	0.020	1
1833	A	11	CYS	N	115.047	0.1	1
1834	C	211	CYS	N	115.047	0.1	1
1835	A	12	ARG	HA	4.028	0.020	1
1836	C	212	ARG	HA	4.028	0.020	1
1837	A	12	ARG	HB2	1.592	0.001	2
1838	C	212	ARG	HB2	1.592	0.001	2
1839	A	12	ARG	HB3	1.528	0.002	2
1840	C	212	ARG	HB3	1.528	0.002	2
1841	A	12	ARG	HD2	3.017	0.020	2
1842	C	212	ARG	HD2	3.017	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1843	A	12	ARG	HD3	3.017	0.020	2
1844	C	212	ARG	HD3	3.017	0.020	2
1845	A	12	ARG	HG2	1.298	0.001	2
1846	C	212	ARG	HG2	1.298	0.001	2
1847	A	12	ARG	HG3	1.197	0.010	2
1848	C	212	ARG	HG3	1.197	0.010	2
1849	A	12	ARG	C	175.097	0.1	1
1850	C	212	ARG	C	175.097	0.1	1
1851	A	12	ARG	CA	57.503	0.1	1
1852	C	212	ARG	CA	57.503	0.1	1
1853	A	12	ARG	CB	31.289	0.1	1
1854	C	212	ARG	CB	31.289	0.1	1
1855	A	12	ARG	CD	43.485	0.1	1
1856	C	212	ARG	CD	43.485	0.1	1
1857	A	12	ARG	CG	26.828	0.066	1
1858	C	212	ARG	CG	26.828	0.066	1
1859	A	13	PHE	H	7.607	0.003	1
1860	C	213	PHE	H	7.607	0.003	1
1861	A	13	PHE	HA	4.497	0.020	1
1862	C	213	PHE	HA	4.497	0.020	1
1863	A	13	PHE	HB2	3.110	0.020	2
1864	C	213	PHE	HB2	3.110	0.020	2
1865	A	13	PHE	HB3	2.818	0.020	2
1866	C	213	PHE	HB3	2.818	0.020	2
1867	A	13	PHE	HD1	7.220	0.020	1
1868	C	213	PHE	HD1	7.220	0.020	1
1869	A	13	PHE	HD2	7.220	0.020	1
1870	C	213	PHE	HD2	7.220	0.020	1
1871	A	13	PHE	HE1	7.350	0.013	1
1872	C	213	PHE	HE1	7.350	0.013	1
1873	A	13	PHE	HE2	7.350	0.013	1
1874	C	213	PHE	HE2	7.350	0.013	1
1875	A	13	PHE	C	174.292	0.1	1
1876	C	213	PHE	C	174.292	0.1	1
1877	A	13	PHE	CA	56.060	0.1	1
1878	C	213	PHE	CA	56.060	0.1	1
1879	A	13	PHE	CB	41.122	0.1	1
1880	C	213	PHE	CB	41.122	0.1	1
1881	A	13	PHE	CD1	132.302	0.1	1
1882	C	213	PHE	CD1	132.302	0.1	1
1883	A	13	PHE	CE1	131.789	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1884	C	213	PHE	CE1	131.789	0.1	1
1885	A	13	PHE	N	116.487	0.1	1
1886	C	213	PHE	N	116.487	0.1	1
1887	A	14	PHE	H	8.202	0.005	1
1888	C	214	PHE	H	8.202	0.005	1
1889	A	14	PHE	HA	4.793	0.006	1
1890	C	214	PHE	HA	4.793	0.006	1
1891	A	14	PHE	HB2	2.770	0.020	2
1892	C	214	PHE	HB2	2.770	0.020	2
1893	A	14	PHE	HB3	2.998	0.020	2
1894	C	214	PHE	HB3	2.998	0.020	2
1895	A	14	PHE	HD1	7.010	0.012	1
1896	C	214	PHE	HD1	7.010	0.012	1
1897	A	14	PHE	HD2	7.010	0.012	1
1898	C	214	PHE	HD2	7.010	0.012	1
1899	A	14	PHE	HE1	7.353	0.020	1
1900	C	214	PHE	HE1	7.353	0.020	1
1901	A	14	PHE	HE2	7.353	0.020	1
1902	C	214	PHE	HE2	7.353	0.020	1
1903	A	14	PHE	C	175.433	0.1	1
1904	C	214	PHE	C	175.433	0.1	1
1905	A	14	PHE	CA	55.516	0.1	1
1906	C	214	PHE	CA	55.516	0.1	1
1907	A	14	PHE	CB	41.096	0.1	1
1908	C	214	PHE	CB	41.096	0.1	1
1909	A	14	PHE	CD1	131.789	0.1	1
1910	C	214	PHE	CD1	131.789	0.1	1
1911	A	14	PHE	CE1	131.789	0.1	1
1912	C	214	PHE	CE1	131.789	0.1	1
1913	A	14	PHE	N	119.591	0.1	1
1914	C	214	PHE	N	119.591	0.1	1
1915	A	15	GLU	H	8.749	0.007	1
1916	C	215	GLU	H	8.749	0.007	1
1917	A	15	GLU	HA	4.579	0.020	1
1918	C	215	GLU	HA	4.579	0.020	1
1919	A	15	GLU	HB2	2.016	0.003	2
1920	C	215	GLU	HB2	2.016	0.003	2
1921	A	15	GLU	HB3	2.154	0.009	2
1922	C	215	GLU	HB3	2.154	0.009	2
1923	A	15	GLU	HG2	2.385	0.006	2
1924	C	215	GLU	HG2	2.385	0.006	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1925	A	15	GLU	HG3	2.385	0.006	2
1926	C	215	GLU	HG3	2.385	0.006	2
1927	A	15	GLU	C	176.809	0.1	1
1928	C	215	GLU	C	176.809	0.1	1
1929	A	15	GLU	CA	56.395	0.1	1
1930	C	215	GLU	CA	56.395	0.1	1
1931	A	15	GLU	CB	30.932	0.1	1
1932	C	215	GLU	CB	30.932	0.1	1
1933	A	15	GLU	CG	36.576	0.1	1
1934	C	215	GLU	CG	36.576	0.1	1
1935	A	15	GLU	N	122.719	0.1	1
1936	C	215	GLU	N	122.719	0.1	1
1937	A	16	SER	H	8.764	0.005	1
1938	C	216	SER	H	8.764	0.005	1
1939	A	16	SER	HA	4.697	0.020	1
1940	C	216	SER	HA	4.697	0.020	1
1941	A	16	SER	HB2	3.858	0.020	2
1942	C	216	SER	HB2	3.858	0.020	2
1943	A	16	SER	HB3	3.772	0.020	2
1944	C	216	SER	HB3	3.772	0.020	2
1945	A	16	SER	CA	59.637	0.1	1
1946	C	216	SER	CA	59.637	0.1	1
1947	A	16	SER	CB	64.708	0.1	1
1948	C	216	SER	CB	64.708	0.1	1
1949	A	16	SER	N	118.765	0.1	1
1950	C	216	SER	N	118.765	0.1	1
1951	A	17	HIS	H	8.617	0.020	1
1952	C	217	HIS	H	8.617	0.020	1
1953	A	17	HIS	HA	4.770	0.020	1
1954	C	217	HIS	HA	4.770	0.020	1
1955	A	17	HIS	HB2	3.222	0.020	2
1956	C	217	HIS	HB2	3.222	0.020	2
1957	A	17	HIS	HB3	3.222	0.020	2
1958	C	217	HIS	HB3	3.222	0.020	2
1959	A	17	HIS	HD2	7.119	0.020	1
1960	C	217	HIS	HD2	7.119	0.020	1
1961	A	17	HIS	HE1	7.963	0.020	1
1962	C	217	HIS	HE1	7.963	0.020	1
1963	A	17	HIS	C	174.658	0.1	1
1964	C	217	HIS	C	174.658	0.1	1
1965	A	17	HIS	CA	56.750	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1966	C	217	HIS	CA	56.750	0.1	1
1967	A	17	HIS	CB	29.718	0.1	1
1968	C	217	HIS	CB	29.718	0.1	1
1969	A	17	HIS	CD2	120.141	0.1	1
1970	C	217	HIS	CD2	120.141	0.1	1
1971	A	17	HIS	CE1	138.518	0.1	1
1972	C	217	HIS	CE1	138.518	0.1	1
1973	A	17	HIS	N	119.651	0.1	1
1974	C	217	HIS	N	119.651	0.1	1
1975	A	18	VAL	H	7.360	0.005	1
1976	C	218	VAL	H	7.360	0.005	1
1977	A	18	VAL	HA	4.100	0.001	1
1978	C	218	VAL	HA	4.100	0.001	1
1979	A	18	VAL	HB	1.957	0.008	1
1980	C	218	VAL	HB	1.957	0.008	1
1981	A	18	VAL	HG11	0.877	0.006	2
1982	C	218	VAL	HG11	0.877	0.006	2
1983	A	18	VAL	HG12	0.877	0.006	2
1984	C	218	VAL	HG12	0.877	0.006	2
1985	A	18	VAL	HG13	0.877	0.006	2
1986	C	218	VAL	HG13	0.877	0.006	2
1987	A	18	VAL	HG21	0.877	0.006	2
1988	C	218	VAL	HG21	0.877	0.006	2
1989	A	18	VAL	HG22	0.877	0.006	2
1990	C	218	VAL	HG22	0.877	0.006	2
1991	A	18	VAL	HG23	0.877	0.006	2
1992	C	218	VAL	HG23	0.877	0.006	2
1993	A	18	VAL	C	174.424	0.1	1
1994	C	218	VAL	C	174.424	0.1	1
1995	A	18	VAL	CA	62.252	0.1	1
1996	C	218	VAL	CA	62.252	0.1	1
1997	A	18	VAL	CB	34.146	0.1	1
1998	C	218	VAL	CB	34.146	0.1	1
1999	A	18	VAL	CG1	22.130	0.1	1
2000	C	218	VAL	CG1	22.130	0.1	1
2001	A	18	VAL	CG2	21.450	0.1	1
2002	C	218	VAL	CG2	21.450	0.1	1
2003	A	18	VAL	N	121.352	0.1	1
2004	C	218	VAL	N	121.352	0.1	1
2005	A	19	ALA	H	8.570	0.006	1
2006	C	219	ALA	H	8.570	0.006	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2007	A	19	ALA	HA	4.345	0.020	1
2008	C	219	ALA	HA	4.345	0.020	1
2009	A	19	ALA	HB1	1.342	0.006	1
2010	C	219	ALA	HB1	1.342	0.006	1
2011	A	19	ALA	HB2	1.342	0.006	1
2012	C	219	ALA	HB2	1.342	0.006	1
2013	A	19	ALA	HB3	1.342	0.006	1
2014	C	219	ALA	HB3	1.342	0.006	1
2015	A	19	ALA	C	177.570	0.1	1
2016	C	219	ALA	C	177.570	0.1	1
2017	A	19	ALA	CA	50.997	0.1	1
2018	C	219	ALA	CA	50.997	0.1	1
2019	A	19	ALA	CB	19.579	0.1	1
2020	C	219	ALA	CB	19.579	0.1	1
2021	A	19	ALA	N	131.401	0.1	1
2022	C	219	ALA	N	131.401	0.1	1
2023	A	20	ARG	H	7.838	0.006	1
2024	C	220	ARG	H	7.838	0.006	1
2025	A	20	ARG	HA	2.545	0.005	1
2026	C	220	ARG	HA	2.545	0.005	1
2027	A	20	ARG	HB2	0.492	0.020	2
2028	C	220	ARG	HB2	0.492	0.020	2
2029	A	20	ARG	HB3	1.035	0.020	2
2030	C	220	ARG	HB3	1.035	0.020	2
2031	A	20	ARG	HD2	2.866	0.001	2
2032	C	220	ARG	HD2	2.866	0.001	2
2033	A	20	ARG	HD3	2.866	0.001	2
2034	C	220	ARG	HD3	2.866	0.001	2
2035	A	20	ARG	HG2	1.176	0.020	2
2036	C	220	ARG	HG2	1.176	0.020	2
2037	A	20	ARG	HG3	0.867	0.004	2
2038	C	220	ARG	HG3	0.867	0.004	2
2039	A	20	ARG	C	178.258	0.1	1
2040	C	220	ARG	C	178.258	0.1	1
2041	A	20	ARG	CA	59.407	0.1	1
2042	C	220	ARG	CA	59.407	0.1	1
2043	A	20	ARG	CB	29.433	0.1	1
2044	C	220	ARG	CB	29.433	0.1	1
2045	A	20	ARG	CD	43.773	0.1	1
2046	C	220	ARG	CD	43.773	0.1	1
2047	A	20	ARG	CG	26.561	0.092	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2048	C	220	ARG	CG	26.561	0.092	1
2049	A	20	ARG	N	124.465	0.1	1
2050	C	220	ARG	N	124.465	0.1	1
2051	A	21	ALA	H	8.203	0.005	1
2052	C	221	ALA	H	8.203	0.005	1
2053	A	21	ALA	HA	4.083	0.020	1
2054	C	221	ALA	HA	4.083	0.020	1
2055	A	21	ALA	HB1	1.302	0.020	1
2056	C	221	ALA	HB1	1.302	0.020	1
2057	A	21	ALA	HB2	1.302	0.020	1
2058	C	221	ALA	HB2	1.302	0.020	1
2059	A	21	ALA	HB3	1.302	0.020	1
2060	C	221	ALA	HB3	1.302	0.020	1
2061	A	21	ALA	C	177.995	0.1	1
2062	C	221	ALA	C	177.995	0.1	1
2063	A	21	ALA	CA	54.000	0.1	1
2064	C	221	ALA	CA	54.000	0.1	1
2065	A	21	ALA	CB	18.722	0.1	1
2066	C	221	ALA	CB	18.722	0.1	1
2067	A	21	ALA	N	117.242	0.1	1
2068	C	221	ALA	N	117.242	0.1	1
2069	A	22	ASN	H	7.739	0.007	1
2070	C	222	ASN	H	7.739	0.007	1
2071	A	22	ASN	HA	4.988	0.008	1
2072	C	222	ASN	HA	4.988	0.008	1
2073	A	22	ASN	HB2	3.100	0.020	2
2074	C	222	ASN	HB2	3.100	0.020	2
2075	A	22	ASN	HB3	2.686	0.003	2
2076	C	222	ASN	HB3	2.686	0.003	2
2077	A	22	ASN	HD21	7.703	0.020	2
2078	C	222	ASN	HD21	7.703	0.020	2
2079	A	22	ASN	HD22	7.133	0.001	2
2080	C	222	ASN	HD22	7.133	0.001	2
2081	A	22	ASN	C	174.848	0.1	1
2082	C	222	ASN	C	174.848	0.1	1
2083	A	22	ASN	CA	52.509	0.009	1
2084	C	222	ASN	CA	52.509	0.009	1
2085	A	22	ASN	CB	40.358	0.1	1
2086	C	222	ASN	CB	40.358	0.1	1
2087	A	22	ASN	N	112.861	0.1	1
2088	C	222	ASN	N	112.861	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2089	A	22	ASN	ND2	112.192	0.1	1
2090	C	222	ASN	ND2	112.192	0.1	1
2091	A	23	VAL	H	7.529	0.013	1
2092	C	223	VAL	H	7.529	0.013	1
2093	A	23	VAL	HA	4.272	0.003	1
2094	C	223	VAL	HA	4.272	0.003	1
2095	A	23	VAL	HB	2.179	0.020	1
2096	C	223	VAL	HB	2.179	0.020	1
2097	A	23	VAL	HG11	0.879	0.020	2
2098	C	223	VAL	HG11	0.879	0.020	2
2099	A	23	VAL	HG12	0.879	0.020	2
2100	C	223	VAL	HG12	0.879	0.020	2
2101	A	23	VAL	HG13	0.879	0.020	2
2102	C	223	VAL	HG13	0.879	0.020	2
2103	A	23	VAL	HG21	0.879	0.020	2
2104	C	223	VAL	HG21	0.879	0.020	2
2105	A	23	VAL	HG22	0.879	0.020	2
2106	C	223	VAL	HG22	0.879	0.020	2
2107	A	23	VAL	HG23	0.879	0.020	2
2108	C	223	VAL	HG23	0.879	0.020	2
2109	A	23	VAL	C	175.755	0.1	1
2110	C	223	VAL	C	175.755	0.1	1
2111	A	23	VAL	CA	62.859	0.1	1
2112	C	223	VAL	CA	62.859	0.1	1
2113	A	23	VAL	CB	33.432	0.1	1
2114	C	223	VAL	CB	33.432	0.1	1
2115	A	23	VAL	CG1	22.794	0.045	1
2116	C	223	VAL	CG1	22.794	0.045	1
2117	A	23	VAL	CG2	22.687	0.1	1
2118	C	223	VAL	CG2	22.687	0.1	1
2119	A	23	VAL	N	119.883	0.1	1
2120	C	223	VAL	N	119.883	0.1	1
2121	A	24	LYS	H	9.527	0.007	1
2122	C	224	LYS	H	9.527	0.007	1
2123	A	24	LYS	HA	4.298	0.020	1
2124	C	224	LYS	HA	4.298	0.020	1
2125	A	24	LYS	HB2	1.267	0.001	2
2126	C	224	LYS	HB2	1.267	0.001	2
2127	A	24	LYS	HB3	1.619	0.009	2
2128	C	224	LYS	HB3	1.619	0.009	2
2129	A	24	LYS	HD2	1.631	0.005	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2130	C	224	LYS	HD2	1.631	0.005	2
2131	A	24	LYS	HD3	1.631	0.005	2
2132	C	224	LYS	HD3	1.631	0.005	2
2133	A	24	LYS	HE2	3.045	0.001	2
2134	C	224	LYS	HE2	3.045	0.001	2
2135	A	24	LYS	HE3	3.045	0.001	2
2136	C	224	LYS	HE3	3.045	0.001	2
2137	A	24	LYS	HG2	1.328	0.002	2
2138	C	224	LYS	HG2	1.328	0.002	2
2139	A	24	LYS	HG3	1.424	0.020	2
2140	C	224	LYS	HG3	1.424	0.020	2
2141	A	24	LYS	C	176.634	0.1	1
2142	C	224	LYS	C	176.634	0.1	1
2143	A	24	LYS	CA	58.989	0.1	1
2144	C	224	LYS	CA	58.989	0.1	1
2145	A	24	LYS	CB	34.390	0.1	1
2146	C	224	LYS	CB	34.390	0.1	1
2147	A	24	LYS	CD	30.263	0.1	1
2148	C	224	LYS	CD	30.263	0.1	1
2149	A	24	LYS	CE	42.132	0.1	1
2150	C	224	LYS	CE	42.132	0.1	1
2151	A	24	LYS	CG	25.843	0.1	1
2152	C	224	LYS	CG	25.843	0.1	1
2153	A	24	LYS	N	128.312	0.1	1
2154	C	224	LYS	N	128.312	0.1	1
2155	A	25	HIS	H	7.214	0.005	1
2156	C	225	HIS	H	7.214	0.005	1
2157	A	25	HIS	HA	4.951	0.003	1
2158	C	225	HIS	HA	4.951	0.003	1
2159	A	25	HIS	HB2	3.655	0.003	2
2160	C	225	HIS	HB2	3.655	0.003	2
2161	A	25	HIS	HB3	3.056	0.010	2
2162	C	225	HIS	HB3	3.056	0.010	2
2163	A	25	HIS	HD2	6.538	0.005	1
2164	C	225	HIS	HD2	6.538	0.005	1
2165	A	25	HIS	HE1	7.874	0.020	1
2166	C	225	HIS	HE1	7.874	0.020	1
2167	A	25	HIS	C	172.740	0.1	1
2168	C	225	HIS	C	172.740	0.1	1
2169	A	25	HIS	CA	55.328	0.1	1
2170	C	225	HIS	CA	55.328	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2171	A	25	HIS	CB	32.882	0.1	1
2172	C	225	HIS	CB	32.882	0.1	1
2173	A	25	HIS	CD2	120.141	0.1	1
2174	C	225	HIS	CD2	120.141	0.1	1
2175	A	25	HIS	CE1	138.518	0.1	1
2176	C	225	HIS	CE1	138.518	0.1	1
2177	A	25	HIS	N	109.505	0.1	1
2178	C	225	HIS	N	109.505	0.1	1
2179	A	26	LEU	H	8.068	0.007	1
2180	C	226	LEU	H	8.068	0.007	1
2181	A	26	LEU	HA	5.182	0.020	1
2182	C	226	LEU	HA	5.182	0.020	1
2183	A	26	LEU	HB2	1.702	0.020	2
2184	C	226	LEU	HB2	1.702	0.020	2
2185	A	26	LEU	HB3	1.245	0.020	2
2186	C	226	LEU	HB3	1.245	0.020	2
2187	A	26	LEU	HD11	0.745	0.008	2
2188	C	226	LEU	HD11	0.745	0.008	2
2189	A	26	LEU	HD12	0.745	0.008	2
2190	C	226	LEU	HD12	0.745	0.008	2
2191	A	26	LEU	HD13	0.745	0.008	2
2192	C	226	LEU	HD13	0.745	0.008	2
2193	A	26	LEU	HD21	0.531	0.005	2
2194	C	226	LEU	HD21	0.531	0.005	2
2195	A	26	LEU	HD22	0.531	0.005	2
2196	C	226	LEU	HD22	0.531	0.005	2
2197	A	26	LEU	HD23	0.531	0.005	2
2198	C	226	LEU	HD23	0.531	0.005	2
2199	A	26	LEU	HG	1.429	0.020	1
2200	C	226	LEU	HG	1.429	0.020	1
2201	A	26	LEU	C	175.346	0.1	1
2202	C	226	LEU	C	175.346	0.1	1
2203	A	26	LEU	CA	53.466	0.1	1
2204	C	226	LEU	CA	53.466	0.1	1
2205	A	26	LEU	CB	45.200	0.1	1
2206	C	226	LEU	CB	45.200	0.1	1
2207	A	26	LEU	CD1	23.949	0.1	1
2208	C	226	LEU	CD1	23.949	0.1	1
2209	A	26	LEU	CD2	26.349	0.1	1
2210	C	226	LEU	CD2	26.349	0.1	1
2211	A	26	LEU	CG	26.601	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2212	C	226	LEU	CG	26.601	0.1	1
2213	A	26	LEU	N	116.963	0.1	1
2214	C	226	LEU	N	116.963	0.1	1
2215	A	27	LYS	H	9.549	0.007	1
2216	C	227	LYS	H	9.549	0.007	1
2217	A	27	LYS	HA	5.374	0.020	1
2218	C	227	LYS	HA	5.374	0.020	1
2219	A	27	LYS	HB2	1.561	0.001	2
2220	C	227	LYS	HB2	1.561	0.001	2
2221	A	27	LYS	HB3	1.561	0.001	2
2222	C	227	LYS	HB3	1.561	0.001	2
2223	A	27	LYS	HD2	1.098	0.020	2
2224	C	227	LYS	HD2	1.098	0.020	2
2225	A	27	LYS	HD3	0.917	0.020	2
2226	C	227	LYS	HD3	0.917	0.020	2
2227	A	27	LYS	HE2	2.446	0.020	2
2228	C	227	LYS	HE2	2.446	0.020	2
2229	A	27	LYS	HE3	2.243	0.001	2
2230	C	227	LYS	HE3	2.243	0.001	2
2231	A	27	LYS	HG2	1.257	0.020	2
2232	C	227	LYS	HG2	1.257	0.020	2
2233	A	27	LYS	HG3	1.040	0.020	2
2234	C	227	LYS	HG3	1.040	0.020	2
2235	A	27	LYS	C	174.716	0.1	1
2236	C	227	LYS	C	174.716	0.1	1
2237	A	27	LYS	CA	55.118	0.1	1
2238	C	227	LYS	CA	55.118	0.1	1
2239	A	27	LYS	CB	35.144	0.1	1
2240	C	227	LYS	CB	35.144	0.1	1
2241	A	27	LYS	CD	29.884	0.1	1
2242	C	227	LYS	CD	29.884	0.1	1
2243	A	27	LYS	CE	41.501	0.1	1
2244	C	227	LYS	CE	41.501	0.1	1
2245	A	27	LYS	CG	25.710	0.052	1
2246	C	227	LYS	CG	25.710	0.052	1
2247	A	27	LYS	N	123.299	0.1	1
2248	C	227	LYS	N	123.299	0.1	1
2249	A	28	ILE	H	9.138	0.006	1
2250	C	228	ILE	H	9.138	0.006	1
2251	A	28	ILE	HA	4.910	0.004	1
2252	C	228	ILE	HA	4.910	0.004	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2253	A	28	ILE	HB	1.861	0.012	1
2254	C	228	ILE	HB	1.861	0.012	1
2255	A	28	ILE	HD11	0.755	0.020	1
2256	C	228	ILE	HD11	0.755	0.020	1
2257	A	28	ILE	HD12	0.755	0.020	1
2258	C	228	ILE	HD12	0.755	0.020	1
2259	A	28	ILE	HD13	0.755	0.020	1
2260	C	228	ILE	HD13	0.755	0.020	1
2261	A	28	ILE	HG12	1.505	0.005	2
2262	C	228	ILE	HG12	1.505	0.005	2
2263	A	28	ILE	HG13	1.149	0.003	2
2264	C	228	ILE	HG13	1.149	0.003	2
2265	A	28	ILE	HG21	0.959	0.020	1
2266	C	228	ILE	HG21	0.959	0.020	1
2267	A	28	ILE	HG22	0.959	0.020	1
2268	C	228	ILE	HG22	0.959	0.020	1
2269	A	28	ILE	HG23	0.959	0.020	1
2270	C	228	ILE	HG23	0.959	0.020	1
2271	A	28	ILE	C	176.970	0.1	1
2272	C	228	ILE	C	176.970	0.1	1
2273	A	28	ILE	CA	60.390	0.1	1
2274	C	228	ILE	CA	60.390	0.1	1
2275	A	28	ILE	CB	39.603	0.1	1
2276	C	228	ILE	CB	39.603	0.1	1
2277	A	28	ILE	CD1	14.101	0.1	1
2278	C	228	ILE	CD1	14.101	0.1	1
2279	A	28	ILE	CG1	27.631	0.1	1
2280	C	228	ILE	CG1	27.631	0.1	1
2281	A	28	ILE	CG2	18.571	0.1	1
2282	C	228	ILE	CG2	18.571	0.1	1
2283	A	28	ILE	N	123.823	0.1	1
2284	C	228	ILE	N	123.823	0.1	1
2285	A	29	LEU	H	8.866	0.005	1
2286	C	229	LEU	H	8.866	0.005	1
2287	A	29	LEU	HA	4.593	0.003	1
2288	C	229	LEU	HA	4.593	0.003	1
2289	A	29	LEU	HB2	1.711	0.001	2
2290	C	229	LEU	HB2	1.711	0.001	2
2291	A	29	LEU	HB3	1.876	0.020	2
2292	C	229	LEU	HB3	1.876	0.020	2
2293	A	29	LEU	HD11	0.912	0.005	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2294	C	229	LEU	HD11	0.912	0.005	2
2295	A	29	LEU	HD12	0.912	0.005	2
2296	C	229	LEU	HD12	0.912	0.005	2
2297	A	29	LEU	HD13	0.912	0.005	2
2298	C	229	LEU	HD13	0.912	0.005	2
2299	A	29	LEU	HD21	0.830	0.020	2
2300	C	229	LEU	HD21	0.830	0.020	2
2301	A	29	LEU	HD22	0.830	0.020	2
2302	C	229	LEU	HD22	0.830	0.020	2
2303	A	29	LEU	HD23	0.830	0.020	2
2304	C	229	LEU	HD23	0.830	0.020	2
2305	A	29	LEU	C	175.975	0.1	1
2306	C	229	LEU	C	175.975	0.1	1
2307	A	29	LEU	CA	55.474	0.1	1
2308	C	229	LEU	CA	55.474	0.1	1
2309	A	29	LEU	CB	42.749	0.1	1
2310	C	229	LEU	CB	42.749	0.1	1
2311	A	29	LEU	CD1	25.591	0.1	1
2312	C	229	LEU	CD1	25.591	0.1	1
2313	A	29	LEU	CD2	23.101	0.1	1
2314	C	229	LEU	CD2	23.101	0.1	1
2315	A	29	LEU	N	128.835	0.1	1
2316	C	229	LEU	N	128.835	0.1	1
2317	A	30	ASN	H	8.211	0.020	1
2318	C	230	ASN	H	8.211	0.020	1
2319	A	30	ASN	HA	4.998	0.020	1
2320	C	230	ASN	HA	4.998	0.020	1
2321	A	30	ASN	HB2	2.389	0.020	2
2322	C	230	ASN	HB2	2.389	0.020	2
2323	A	30	ASN	HB3	2.903	0.020	2
2324	C	230	ASN	HB3	2.903	0.020	2
2325	A	30	ASN	HD21	7.629	0.004	2
2326	C	230	ASN	HD21	7.629	0.004	2
2327	A	30	ASN	HD22	6.295	0.003	2
2328	C	230	ASN	HD22	6.295	0.003	2
2329	A	30	ASN	C	174.658	0.1	1
2330	C	230	ASN	C	174.658	0.1	1
2331	A	30	ASN	CA	52.524	0.1	1
2332	C	230	ASN	CA	52.524	0.1	1
2333	A	30	ASN	CB	38.978	0.1	1
2334	C	230	ASN	CB	38.978	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2335	A	30	ASN	N	120.696	0.1	1
2336	C	230	ASN	N	120.696	0.1	1
2337	A	30	ASN	ND2	111.827	0.016	1
2338	C	230	ASN	ND2	111.827	0.016	1
2339	A	31	THR	H	7.925	0.020	1
2340	C	231	THR	H	7.925	0.020	1
2341	A	31	THR	HA	4.784	0.003	1
2342	C	231	THR	HA	4.784	0.003	1
2343	A	31	THR	HB	4.159	0.004	1
2344	C	231	THR	HB	4.159	0.004	1
2345	A	31	THR	HG21	1.210	0.004	1
2346	C	231	THR	HG21	1.210	0.004	1
2347	A	31	THR	HG22	1.210	0.004	1
2348	C	231	THR	HG22	1.210	0.004	1
2349	A	31	THR	HG23	1.210	0.004	1
2350	C	231	THR	HG23	1.210	0.004	1
2351	A	31	THR	CA	58.046	0.1	1
2352	C	231	THR	CA	58.046	0.1	1
2353	A	31	THR	CB	70.341	0.1	1
2354	C	231	THR	CB	70.341	0.1	1
2355	A	31	THR	CG2	22.130	0.1	1
2356	C	231	THR	CG2	22.130	0.1	1
2357	A	31	THR	N	116.303	0.1	1
2358	C	231	THR	N	116.303	0.1	1
2359	A	32	PRO	HA	4.300	0.002	1
2360	C	232	PRO	HA	4.300	0.002	1
2361	A	32	PRO	HB2	2.346	0.020	2
2362	C	232	PRO	HB2	2.346	0.020	2
2363	A	32	PRO	HB3	1.876	0.019	2
2364	C	232	PRO	HB3	1.876	0.019	2
2365	A	32	PRO	HD2	3.758	0.003	2
2366	C	232	PRO	HD2	3.758	0.003	2
2367	A	32	PRO	HD3	3.758	0.003	2
2368	C	232	PRO	HD3	3.758	0.003	2
2369	A	32	PRO	HG2	2.085	0.001	2
2370	C	232	PRO	HG2	2.085	0.001	2
2371	A	32	PRO	HG3	1.965	0.020	2
2372	C	232	PRO	HG3	1.965	0.020	2
2373	A	32	PRO	C	176.765	0.1	1
2374	C	232	PRO	C	176.765	0.1	1
2375	A	32	PRO	CA	65.164	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2376	C	232	PRO	CA	65.164	0.1	1
2377	A	32	PRO	CB	32.484	0.1	1
2378	C	232	PRO	CB	32.484	0.1	1
2379	A	32	PRO	CD	51.251	0.1	1
2380	C	232	PRO	CD	51.251	0.1	1
2381	A	32	PRO	CG	27.631	0.1	1
2382	C	232	PRO	CG	27.631	0.1	1
2383	A	33	ASN	H	8.294	0.003	1
2384	C	233	ASN	H	8.294	0.003	1
2385	A	33	ASN	C	174.541	0.1	1
2386	C	233	ASN	C	174.541	0.1	1
2387	A	33	ASN	N	120.212	0.082	1
2388	C	233	ASN	N	120.212	0.082	1
2389	A	34	CYS	H	7.561	0.008	1
2390	C	234	CYS	H	7.561	0.008	1
2391	A	34	CYS	HA	4.884	0.020	1
2392	C	234	CYS	HA	4.884	0.020	1
2393	A	34	CYS	HB2	3.141	0.002	2
2394	C	234	CYS	HB2	3.141	0.002	2
2395	A	34	CYS	HB3	2.970	0.005	2
2396	C	234	CYS	HB3	2.970	0.005	2
2397	A	34	CYS	C	173.838	0.1	1
2398	C	234	CYS	C	173.838	0.1	1
2399	A	34	CYS	CA	55.139	0.1	1
2400	C	234	CYS	CA	55.139	0.1	1
2401	A	34	CYS	CB	45.200	0.1	1
2402	C	234	CYS	CB	45.200	0.1	1
2403	A	34	CYS	N	116.986	0.040	1
2404	C	234	CYS	N	116.986	0.040	1
2405	A	35	ALA	H	8.520	0.020	1
2406	C	235	ALA	H	8.520	0.020	1
2407	A	35	ALA	HA	4.233	0.020	1
2408	C	235	ALA	HA	4.233	0.020	1
2409	A	35	ALA	HB1	1.440	0.020	1
2410	C	235	ALA	HB1	1.440	0.020	1
2411	A	35	ALA	HB2	1.440	0.020	1
2412	C	235	ALA	HB2	1.440	0.020	1
2413	A	35	ALA	HB3	1.440	0.020	1
2414	C	235	ALA	HB3	1.440	0.020	1
2415	A	35	ALA	C	176.326	0.1	1
2416	C	235	ALA	C	176.326	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2417	A	35	ALA	CA	53.152	0.1	1
2418	C	235	ALA	CA	53.152	0.1	1
2419	A	35	ALA	CB	18.930	0.1	1
2420	C	235	ALA	CB	18.930	0.1	1
2421	A	35	ALA	N	125.167	0.1	1
2422	C	235	ALA	N	125.167	0.1	1
2423	A	36	CYS	H	8.343	0.020	1
2424	C	236	CYS	H	8.343	0.020	1
2425	A	36	CYS	HA	4.213	0.002	1
2426	C	236	CYS	HA	4.213	0.002	1
2427	A	36	CYS	HB2	2.652	0.012	2
2428	C	236	CYS	HB2	2.652	0.012	2
2429	A	36	CYS	HB3	3.480	0.020	2
2430	C	236	CYS	HB3	3.480	0.020	2
2431	A	36	CYS	C	173.589	0.1	1
2432	C	236	CYS	C	173.589	0.1	1
2433	A	36	CYS	CA	58.487	0.062	1
2434	C	236	CYS	CA	58.487	0.062	1
2435	A	36	CYS	CB	45.702	0.1	1
2436	C	236	CYS	CB	45.702	0.1	1
2437	A	36	CYS	N	118.786	0.1	1
2438	C	236	CYS	N	118.786	0.1	1
2439	A	37	GLN	H	8.988	0.005	1
2440	C	237	GLN	H	8.988	0.005	1
2441	A	37	GLN	HA	4.573	0.020	1
2442	C	237	GLN	HA	4.573	0.020	1
2443	A	37	GLN	HB2	2.314	0.004	2
2444	C	237	GLN	HB2	2.314	0.004	2
2445	A	37	GLN	HB3	1.827	0.020	2
2446	C	237	GLN	HB3	1.827	0.020	2
2447	A	37	GLN	HE21	7.264	0.003	2
2448	C	237	GLN	HE21	7.264	0.003	2
2449	A	37	GLN	HE22	6.894	0.002	2
2450	C	237	GLN	HE22	6.894	0.002	2
2451	A	37	GLN	HG2	2.589	0.009	2
2452	C	237	GLN	HG2	2.589	0.009	2
2453	A	37	GLN	HG3	2.306	0.007	2
2454	C	237	GLN	HG3	2.306	0.007	2
2455	A	37	GLN	C	173.545	0.1	1
2456	C	237	GLN	C	173.545	0.1	1
2457	A	37	GLN	CA	54.491	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2458	C	237	GLN	CA	54.491	0.1	1
2459	A	37	GLN	CB	31.876	0.1	1
2460	C	237	GLN	CB	31.876	0.1	1
2461	A	37	GLN	CG	34.426	0.1	1
2462	C	237	GLN	CG	34.426	0.1	1
2463	A	37	GLN	N	128.825	0.1	1
2464	C	237	GLN	N	128.825	0.1	1
2465	A	37	GLN	NE2	113.029	0.001	1
2466	C	237	GLN	NE2	113.029	0.001	1
2467	A	38	ILE	H	8.967	0.020	1
2468	C	238	ILE	H	8.967	0.020	1
2469	A	38	ILE	HA	5.095	0.004	1
2470	C	238	ILE	HA	5.095	0.004	1
2471	A	38	ILE	HB	1.770	0.007	1
2472	C	238	ILE	HB	1.770	0.007	1
2473	A	38	ILE	HD11	0.715	0.003	1
2474	C	238	ILE	HD11	0.715	0.003	1
2475	A	38	ILE	HD12	0.715	0.003	1
2476	C	238	ILE	HD12	0.715	0.003	1
2477	A	38	ILE	HD13	0.715	0.003	1
2478	C	238	ILE	HD13	0.715	0.003	1
2479	A	38	ILE	HG12	0.973	0.003	2
2480	C	238	ILE	HG12	0.973	0.003	2
2481	A	38	ILE	HG13	0.973	0.003	2
2482	C	238	ILE	HG13	0.973	0.003	2
2483	A	38	ILE	HG21	0.723	0.008	1
2484	C	238	ILE	HG21	0.723	0.008	1
2485	A	38	ILE	HG22	0.723	0.008	1
2486	C	238	ILE	HG22	0.723	0.008	1
2487	A	38	ILE	HG23	0.723	0.008	1
2488	C	238	ILE	HG23	0.723	0.008	1
2489	A	38	ILE	C	174.336	0.1	1
2490	C	238	ILE	C	174.336	0.1	1
2491	A	38	ILE	CA	60.620	0.1	1
2492	C	238	ILE	CA	60.620	0.1	1
2493	A	38	ILE	CB	40.235	0.1	1
2494	C	238	ILE	CB	40.235	0.1	1
2495	A	38	ILE	CD1	14.101	0.1	1
2496	C	238	ILE	CD1	14.101	0.1	1
2497	A	38	ILE	CG1	28.243	0.1	1
2498	C	238	ILE	CG1	28.243	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2499	A	38	ILE	CG2	19.278	0.1	1
2500	C	238	ILE	CG2	19.278	0.1	1
2501	A	38	ILE	N	124.006	0.1	1
2502	C	238	ILE	N	124.006	0.1	1
2503	A	39	VAL	H	9.130	0.009	1
2504	C	239	VAL	H	9.130	0.009	1
2505	A	39	VAL	HA	4.926	0.008	1
2506	C	239	VAL	HA	4.926	0.008	1
2507	A	39	VAL	HB	1.795	0.002	1
2508	C	239	VAL	HB	1.795	0.002	1
2509	A	39	VAL	HG11	0.905	0.003	2
2510	C	239	VAL	HG11	0.905	0.003	2
2511	A	39	VAL	HG12	0.905	0.003	2
2512	C	239	VAL	HG12	0.905	0.003	2
2513	A	39	VAL	HG13	0.905	0.003	2
2514	C	239	VAL	HG13	0.905	0.003	2
2515	A	39	VAL	HG21	0.842	0.007	2
2516	C	239	VAL	HG21	0.842	0.007	2
2517	A	39	VAL	HG22	0.842	0.007	2
2518	C	239	VAL	HG22	0.842	0.007	2
2519	A	39	VAL	HG23	0.842	0.007	2
2520	C	239	VAL	HG23	0.842	0.007	2
2521	A	39	VAL	C	175.492	0.1	1
2522	C	239	VAL	C	175.492	0.1	1
2523	A	39	VAL	CA	59.993	0.1	1
2524	C	239	VAL	CA	59.993	0.1	1
2525	A	39	VAL	CB	35.270	0.1	1
2526	C	239	VAL	CB	35.270	0.1	1
2527	A	39	VAL	CG1	21.483	0.1	1
2528	C	239	VAL	CG1	21.483	0.1	1
2529	A	39	VAL	CG2	22.454	0.1	1
2530	C	239	VAL	CG2	22.454	0.1	1
2531	A	39	VAL	N	125.973	0.1	1
2532	C	239	VAL	N	125.973	0.1	1
2533	A	40	ALA	H	9.558	0.005	1
2534	C	240	ALA	H	9.558	0.005	1
2535	A	40	ALA	HA	5.123	0.008	1
2536	C	240	ALA	HA	5.123	0.008	1
2537	A	40	ALA	HB1	1.319	0.006	1
2538	C	240	ALA	HB1	1.319	0.006	1
2539	A	40	ALA	HB2	1.319	0.006	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2540	C	240	ALA	HB2	1.319	0.006	1
2541	A	40	ALA	HB3	1.319	0.006	1
2542	C	240	ALA	HB3	1.319	0.006	1
2543	A	40	ALA	C	175.931	0.1	1
2544	C	240	ALA	C	175.931	0.1	1
2545	A	40	ALA	CA	50.558	0.1	1
2546	C	240	ALA	CA	50.558	0.1	1
2547	A	40	ALA	CB	22.072	0.1	1
2548	C	240	ALA	CB	22.072	0.1	1
2549	A	40	ALA	N	128.264	0.1	1
2550	C	240	ALA	N	128.264	0.1	1
2551	A	41	ARG	H	7.707	0.008	1
2552	C	241	ARG	H	7.707	0.008	1
2553	A	41	ARG	HA	4.966	0.004	1
2554	C	241	ARG	HA	4.966	0.004	1
2555	A	41	ARG	HB2	1.434	0.020	2
2556	C	241	ARG	HB2	1.434	0.020	2
2557	A	41	ARG	HB3	0.944	0.007	2
2558	C	241	ARG	HB3	0.944	0.007	2
2559	A	41	ARG	HD2	3.081	0.003	2
2560	C	241	ARG	HD2	3.081	0.003	2
2561	A	41	ARG	HD3	3.081	0.003	2
2562	C	241	ARG	HD3	3.081	0.003	2
2563	A	41	ARG	HG2	1.506	0.008	2
2564	C	241	ARG	HG2	1.506	0.008	2
2565	A	41	ARG	HG3	1.379	0.007	2
2566	C	241	ARG	HG3	1.379	0.007	2
2567	A	41	ARG	C	175.477	0.1	1
2568	C	241	ARG	C	175.477	0.1	1
2569	A	41	ARG	CA	54.000	0.1	1
2570	C	241	ARG	CA	54.000	0.1	1
2571	A	41	ARG	CB	31.122	0.1	1
2572	C	241	ARG	CB	31.122	0.1	1
2573	A	41	ARG	CD	42.400	0.043	1
2574	C	241	ARG	CD	42.400	0.043	1
2575	A	41	ARG	CG	27.307	0.1	1
2576	C	241	ARG	CG	27.307	0.1	1
2577	A	41	ARG	N	121.647	0.1	1
2578	C	241	ARG	N	121.647	0.1	1
2579	A	42	LEU	H	9.183	0.007	1
2580	C	242	LEU	H	9.183	0.007	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2581	A	42	LEU	HA	5.009	0.007	1
2582	C	242	LEU	HA	5.009	0.007	1
2583	A	42	LEU	HB2	2.180	0.002	2
2584	C	242	LEU	HB2	2.180	0.002	2
2585	A	42	LEU	HB3	1.771	0.008	2
2586	C	242	LEU	HB3	1.771	0.008	2
2587	A	42	LEU	HD11	1.005	0.007	2
2588	C	242	LEU	HD11	1.005	0.007	2
2589	A	42	LEU	HD12	1.005	0.007	2
2590	C	242	LEU	HD12	1.005	0.007	2
2591	A	42	LEU	HD13	1.005	0.007	2
2592	C	242	LEU	HD13	1.005	0.007	2
2593	A	42	LEU	HD21	0.775	0.001	2
2594	C	242	LEU	HD21	0.775	0.001	2
2595	A	42	LEU	HD22	0.775	0.001	2
2596	C	242	LEU	HD22	0.775	0.001	2
2597	A	42	LEU	HD23	0.775	0.001	2
2598	C	242	LEU	HD23	0.775	0.001	2
2599	A	42	LEU	HG	1.787	0.006	1
2600	C	242	LEU	HG	1.787	0.006	1
2601	A	42	LEU	C	177.848	0.1	1
2602	C	242	LEU	C	177.848	0.1	1
2603	A	42	LEU	CA	54.596	0.1	1
2604	C	242	LEU	CA	54.596	0.1	1
2605	A	42	LEU	CB	41.806	0.1	1
2606	C	242	LEU	CB	41.806	0.1	1
2607	A	42	LEU	CD1	25.843	0.1	1
2608	C	242	LEU	CD1	25.843	0.1	1
2609	A	42	LEU	CD2	23.192	0.1	1
2610	C	242	LEU	CD2	23.192	0.1	1
2611	A	42	LEU	CG	27.716	0.042	1
2612	C	242	LEU	CG	27.716	0.042	1
2613	A	42	LEU	N	128.821	0.1	1
2614	C	242	LEU	N	128.821	0.1	1
2615	A	43	LYS	H	8.449	0.016	1
2616	C	243	LYS	H	8.449	0.016	1
2617	A	43	LYS	N	119.659	0.1	1
2618	C	243	LYS	N	119.659	0.1	1
2619	A	46	ASN	HA	4.716	0.020	1
2620	C	246	ASN	HA	4.716	0.020	1
2621	A	46	ASN	HB2	3.138	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2622	C	246	ASN	HB2	3.138	0.020	2
2623	A	46	ASN	HB3	2.742	0.020	2
2624	C	246	ASN	HB3	2.742	0.020	2
2625	A	46	ASN	HD21	7.628	0.002	2
2626	C	246	ASN	HD21	7.628	0.002	2
2627	A	46	ASN	HD22	6.966	0.001	2
2628	C	246	ASN	HD22	6.966	0.001	2
2629	A	46	ASN	C	175.155	0.1	1
2630	C	246	ASN	C	175.155	0.1	1
2631	A	46	ASN	CA	54.616	0.1	1
2632	C	246	ASN	CA	54.616	0.1	1
2633	A	46	ASN	CB	39.292	0.1	1
2634	C	246	ASN	CB	39.292	0.1	1
2635	A	46	ASN	ND2	113.245	0.1	1
2636	C	246	ASN	ND2	113.245	0.1	1
2637	A	47	ARG	H	7.926	0.005	1
2638	C	247	ARG	H	7.926	0.005	1
2639	A	47	ARG	HA	4.274	0.020	1
2640	C	247	ARG	HA	4.274	0.020	1
2641	A	47	ARG	HB2	1.767	0.001	2
2642	C	247	ARG	HB2	1.767	0.001	2
2643	A	47	ARG	HB3	1.767	0.001	2
2644	C	247	ARG	HB3	1.767	0.001	2
2645	A	47	ARG	HD2	3.238	0.020	2
2646	C	247	ARG	HD2	3.238	0.020	2
2647	A	47	ARG	HD3	3.173	0.001	2
2648	C	247	ARG	HD3	3.173	0.001	2
2649	A	47	ARG	HG2	1.650	0.001	2
2650	C	247	ARG	HG2	1.650	0.001	2
2651	A	47	ARG	HG3	1.573	0.020	2
2652	C	247	ARG	HG3	1.573	0.020	2
2653	A	47	ARG	C	175.433	0.1	1
2654	C	247	ARG	C	175.433	0.1	1
2655	A	47	ARG	CA	57.252	0.1	1
2656	C	247	ARG	CA	57.252	0.1	1
2657	A	47	ARG	CB	32.128	0.1	1
2658	C	247	ARG	CB	32.128	0.1	1
2659	A	47	ARG	CD	43.900	0.1	1
2660	C	247	ARG	CD	43.900	0.1	1
2661	A	47	ARG	CG	28.278	0.1	1
2662	C	247	ARG	CG	28.278	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2663	A	47	ARG	N	120.086	0.1	1
2664	C	247	ARG	N	120.086	0.1	1
2665	A	48	GLN	H	8.542	0.010	1
2666	C	248	GLN	H	8.542	0.010	1
2667	A	48	GLN	HA	5.478	0.003	1
2668	C	248	GLN	HA	5.478	0.003	1
2669	A	48	GLN	HB2	1.876	0.001	2
2670	C	248	GLN	HB2	1.876	0.001	2
2671	A	48	GLN	HB3	1.876	0.001	2
2672	C	248	GLN	HB3	1.876	0.001	2
2673	A	48	GLN	HG2	2.356	0.002	2
2674	C	248	GLN	HG2	2.356	0.002	2
2675	A	48	GLN	HG3	1.973	0.020	2
2676	C	248	GLN	HG3	1.973	0.020	2
2677	A	48	GLN	C	175.697	0.1	1
2678	C	248	GLN	C	175.697	0.1	1
2679	A	48	GLN	CA	55.077	0.1	1
2680	C	248	GLN	CA	55.077	0.1	1
2681	A	48	GLN	CB	31.751	0.1	1
2682	C	248	GLN	CB	31.751	0.1	1
2683	A	48	GLN	CG	35.692	0.1	1
2684	C	248	GLN	CG	35.692	0.1	1
2685	A	48	GLN	N	120.774	0.1	1
2686	C	248	GLN	N	120.774	0.1	1
2687	A	49	VAL	H	8.710	0.009	1
2688	C	249	VAL	H	8.710	0.009	1
2689	A	49	VAL	HA	4.781	0.001	1
2690	C	249	VAL	HA	4.781	0.001	1
2691	A	49	VAL	HB	2.177	0.020	1
2692	C	249	VAL	HB	2.177	0.020	1
2693	A	49	VAL	HG11	0.940	0.009	2
2694	C	249	VAL	HG11	0.940	0.009	2
2695	A	49	VAL	HG12	0.940	0.009	2
2696	C	249	VAL	HG12	0.940	0.009	2
2697	A	49	VAL	HG13	0.940	0.009	2
2698	C	249	VAL	HG13	0.940	0.009	2
2699	A	49	VAL	HG21	0.915	0.002	2
2700	C	249	VAL	HG21	0.915	0.002	2
2701	A	49	VAL	HG22	0.915	0.002	2
2702	C	249	VAL	HG22	0.915	0.002	2
2703	A	49	VAL	HG23	0.915	0.002	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2704	C	249	VAL	HG23	0.915	0.002	2
2705	A	49	VAL	C	175.185	0.1	1
2706	C	249	VAL	C	175.185	0.1	1
2707	A	49	VAL	CA	59.344	0.1	1
2708	C	249	VAL	CA	59.344	0.1	1
2709	A	49	VAL	CB	36.024	0.1	1
2710	C	249	VAL	CB	36.024	0.1	1
2711	A	49	VAL	CG1	21.803	0.1	1
2712	C	249	VAL	CG1	21.803	0.1	1
2713	A	49	VAL	CG2	19.783	0.1	1
2714	C	249	VAL	CG2	19.783	0.1	1
2715	A	49	VAL	N	117.392	0.1	1
2716	C	249	VAL	N	117.392	0.1	1
2717	A	50	CYS	H	9.184	0.012	1
2718	C	250	CYS	H	9.184	0.012	1
2719	A	50	CYS	HA	5.313	0.007	1
2720	C	250	CYS	HA	5.313	0.007	1
2721	A	50	CYS	HB2	3.631	0.003	2
2722	C	250	CYS	HB2	3.631	0.003	2
2723	A	50	CYS	HB3	2.996	0.002	2
2724	C	250	CYS	HB3	2.996	0.002	2
2725	A	50	CYS	C	174.380	0.1	1
2726	C	250	CYS	C	174.380	0.1	1
2727	A	50	CYS	CA	57.984	0.1	1
2728	C	250	CYS	CA	57.984	0.1	1
2729	A	50	CYS	CB	42.661	0.115	1
2730	C	250	CYS	CB	42.661	0.115	1
2731	A	50	CYS	N	124.238	0.1	1
2732	C	250	CYS	N	124.238	0.1	1
2733	A	51	ILE	H	8.434	0.006	1
2734	C	251	ILE	H	8.434	0.006	1
2735	A	51	ILE	HA	4.930	0.014	1
2736	C	251	ILE	HA	4.930	0.014	1
2737	A	51	ILE	HB	1.540	0.006	1
2738	C	251	ILE	HB	1.540	0.006	1
2739	A	51	ILE	HD11	0.743	0.003	1
2740	C	251	ILE	HD11	0.743	0.003	1
2741	A	51	ILE	HD12	0.743	0.003	1
2742	C	251	ILE	HD12	0.743	0.003	1
2743	A	51	ILE	HD13	0.743	0.003	1
2744	C	251	ILE	HD13	0.743	0.003	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2745	A	51	ILE	HG12	1.334	0.003	2
2746	C	251	ILE	HG12	1.334	0.003	2
2747	A	51	ILE	HG13	1.166	0.007	2
2748	C	251	ILE	HG13	1.166	0.007	2
2749	A	51	ILE	HG21	0.740	0.008	1
2750	C	251	ILE	HG21	0.740	0.008	1
2751	A	51	ILE	HG22	0.740	0.008	1
2752	C	251	ILE	HG22	0.740	0.008	1
2753	A	51	ILE	HG23	0.740	0.008	1
2754	C	251	ILE	HG23	0.740	0.008	1
2755	A	51	ILE	C	172.931	0.1	1
2756	C	251	ILE	C	172.931	0.1	1
2757	A	51	ILE	CA	58.675	0.1	1
2758	C	251	ILE	CA	58.675	0.1	1
2759	A	51	ILE	CB	42.309	0.1	1
2760	C	251	ILE	CB	42.309	0.1	1
2761	A	51	ILE	CD1	14.858	0.1	1
2762	C	251	ILE	CD1	14.858	0.1	1
2763	A	51	ILE	CG1	27.733	0.021	1
2764	C	251	ILE	CG1	27.733	0.021	1
2765	A	51	ILE	CG2	18.141	0.1	1
2766	C	251	ILE	CG2	18.141	0.1	1
2767	A	51	ILE	N	122.034	0.1	1
2768	C	251	ILE	N	122.034	0.1	1
2769	A	52	ASP	H	7.702	0.006	1
2770	C	252	ASP	H	7.702	0.006	1
2771	A	52	ASP	HA	3.426	0.020	1
2772	C	252	ASP	HA	3.426	0.020	1
2773	A	52	ASP	HB2	2.662	0.020	2
2774	C	252	ASP	HB2	2.662	0.020	2
2775	A	52	ASP	HB3	2.203	0.020	2
2776	C	252	ASP	HB3	2.203	0.020	2
2777	A	52	ASP	CA	51.251	0.1	1
2778	C	252	ASP	CA	51.251	0.1	1
2779	A	52	ASP	CB	42.515	0.1	1
2780	C	252	ASP	CB	42.515	0.1	1
2781	A	52	ASP	N	125.815	0.1	1
2782	C	252	ASP	N	125.815	0.1	1
2783	A	53	PRO	HA	3.986	0.002	1
2784	C	253	PRO	HA	3.986	0.002	1
2785	A	53	PRO	HB2	2.172	0.002	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2786	C	253	PRO	HB2	2.172	0.002	2
2787	A	53	PRO	HB3	1.889	0.003	2
2788	C	253	PRO	HB3	1.889	0.003	2
2789	A	53	PRO	HD2	3.426	0.020	2
2790	C	253	PRO	HD2	3.426	0.020	2
2791	A	53	PRO	HD3	3.426	0.020	2
2792	C	253	PRO	HD3	3.426	0.020	2
2793	A	53	PRO	HG2	1.895	0.020	2
2794	C	253	PRO	HG2	1.895	0.020	2
2795	A	53	PRO	HG3	1.794	0.005	2
2796	C	253	PRO	HG3	1.794	0.005	2
2797	A	53	PRO	C	176.034	0.1	1
2798	C	253	PRO	C	176.034	0.1	1
2799	A	53	PRO	CA	63.947	0.1	1
2800	C	253	PRO	CA	63.947	0.1	1
2801	A	53	PRO	CB	33.000	0.1	1
2802	C	253	PRO	CB	33.000	0.1	1
2803	A	53	PRO	CD	51.251	0.1	1
2804	C	253	PRO	CD	51.251	0.1	1
2805	A	53	PRO	CG	27.643	0.033	1
2806	C	253	PRO	CG	27.643	0.033	1
2807	A	54	LYS	H	7.889	0.008	1
2808	C	254	LYS	H	7.889	0.008	1
2809	A	54	LYS	HA	3.993	0.001	1
2810	C	254	LYS	HA	3.993	0.001	1
2811	A	54	LYS	HB2	1.760	0.001	2
2812	C	254	LYS	HB2	1.760	0.001	2
2813	A	54	LYS	HB3	1.760	0.001	2
2814	C	254	LYS	HB3	1.760	0.001	2
2815	A	54	LYS	HD2	1.682	0.020	2
2816	C	254	LYS	HD2	1.682	0.020	2
2817	A	54	LYS	HD3	1.682	0.020	2
2818	C	254	LYS	HD3	1.682	0.020	2
2819	A	54	LYS	HE2	3.019	0.020	2
2820	C	254	LYS	HE2	3.019	0.020	2
2821	A	54	LYS	HE3	3.019	0.020	2
2822	C	254	LYS	HE3	3.019	0.020	2
2823	A	54	LYS	HG2	1.408	0.002	2
2824	C	254	LYS	HG2	1.408	0.002	2
2825	A	54	LYS	HG3	1.333	0.020	2
2826	C	254	LYS	HG3	1.333	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2827	A	54	LYS	C	177.922	0.1	1
2828	C	254	LYS	C	177.922	0.1	1
2829	A	54	LYS	CA	56.729	0.1	1
2830	C	254	LYS	CA	56.729	0.1	1
2831	A	54	LYS	CB	31.751	0.1	1
2832	C	254	LYS	CB	31.751	0.1	1
2833	A	54	LYS	CD	29.000	0.1	1
2834	C	254	LYS	CD	29.000	0.1	1
2835	A	54	LYS	CE	41.753	0.1	1
2836	C	254	LYS	CE	41.753	0.1	1
2837	A	54	LYS	CG	25.212	0.1	1
2838	C	254	LYS	CG	25.212	0.1	1
2839	A	54	LYS	N	112.456	0.1	1
2840	C	254	LYS	N	112.456	0.1	1
2841	A	55	LEU	H	7.157	0.008	1
2842	C	255	LEU	H	7.157	0.008	1
2843	A	55	LEU	HA	4.040	0.020	1
2844	C	255	LEU	HA	4.040	0.020	1
2845	A	55	LEU	HB2	1.246	0.002	2
2846	C	255	LEU	HB2	1.246	0.002	2
2847	A	55	LEU	HB3	1.064	0.004	2
2848	C	255	LEU	HB3	1.064	0.004	2
2849	A	55	LEU	HD11	1.068	0.004	2
2850	C	255	LEU	HD11	1.068	0.004	2
2851	A	55	LEU	HD12	1.068	0.004	2
2852	C	255	LEU	HD12	1.068	0.004	2
2853	A	55	LEU	HD13	1.068	0.004	2
2854	C	255	LEU	HD13	1.068	0.004	2
2855	A	55	LEU	HD21	1.060	0.003	2
2856	C	255	LEU	HD21	1.060	0.003	2
2857	A	55	LEU	HD22	1.060	0.003	2
2858	C	255	LEU	HD22	1.060	0.003	2
2859	A	55	LEU	HD23	1.060	0.003	2
2860	C	255	LEU	HD23	1.060	0.003	2
2861	A	55	LEU	HG	1.907	0.008	1
2862	C	255	LEU	HG	1.907	0.008	1
2863	A	55	LEU	C	179.268	0.1	1
2864	C	255	LEU	C	179.268	0.1	1
2865	A	55	LEU	CA	55.997	0.1	1
2866	C	255	LEU	CA	55.997	0.1	1
2867	A	55	LEU	CB	42.309	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2868	C	255	LEU	CB	42.309	0.1	1
2869	A	55	LEU	CD1	25.717	0.1	1
2870	C	255	LEU	CD1	25.717	0.1	1
2871	A	55	LEU	CD2	23.318	0.1	1
2872	C	255	LEU	CD2	23.318	0.1	1
2873	A	55	LEU	CG	26.878	0.050	1
2874	C	255	LEU	CG	26.878	0.050	1
2875	A	55	LEU	N	120.452	0.1	1
2876	C	255	LEU	N	120.452	0.1	1
2877	A	56	LYS	H	8.731	0.004	1
2878	C	256	LYS	H	8.731	0.004	1
2879	A	56	LYS	HA	3.913	0.005	1
2880	C	256	LYS	HA	3.913	0.005	1
2881	A	56	LYS	HB2	2.018	0.020	2
2882	C	256	LYS	HB2	2.018	0.020	2
2883	A	56	LYS	HB3	2.018	0.020	2
2884	C	256	LYS	HB3	2.018	0.020	2
2885	A	56	LYS	HD2	1.801	0.003	2
2886	C	256	LYS	HD2	1.801	0.003	2
2887	A	56	LYS	HD3	1.801	0.003	2
2888	C	256	LYS	HD3	1.801	0.003	2
2889	A	56	LYS	HE2	3.080	0.010	2
2890	C	256	LYS	HE2	3.080	0.010	2
2891	A	56	LYS	HE3	3.080	0.010	2
2892	C	256	LYS	HE3	3.080	0.010	2
2893	A	56	LYS	HG2	1.578	0.006	2
2894	C	256	LYS	HG2	1.578	0.006	2
2895	A	56	LYS	HG3	1.578	0.006	2
2896	C	256	LYS	HG3	1.578	0.006	2
2897	A	56	LYS	C	178.917	0.1	1
2898	C	256	LYS	C	178.917	0.1	1
2899	A	56	LYS	CA	60.202	0.1	1
2900	C	256	LYS	CA	60.202	0.1	1
2901	A	56	LYS	CB	32.253	0.1	1
2902	C	256	LYS	CB	32.253	0.1	1
2903	A	56	LYS	CD	29.379	0.1	1
2904	C	256	LYS	CD	29.379	0.1	1
2905	A	56	LYS	CE	42.515	0.1	1
2906	C	256	LYS	CE	42.515	0.1	1
2907	A	56	LYS	CG	25.086	0.1	1
2908	C	256	LYS	CG	25.086	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2909	A	56	LYS	N	125.307	0.1	1
2910	C	256	LYS	N	125.307	0.1	1
2911	A	57	TRP	H	7.884	0.020	1
2912	C	257	TRP	H	7.884	0.020	1
2913	A	57	TRP	HA	4.637	0.002	1
2914	C	257	TRP	HA	4.637	0.002	1
2915	A	57	TRP	HB2	3.628	0.006	2
2916	C	257	TRP	HB2	3.628	0.006	2
2917	A	57	TRP	HB3	3.298	0.001	2
2918	C	257	TRP	HB3	3.298	0.001	2
2919	A	57	TRP	HD1	7.734	0.005	1
2920	C	257	TRP	HD1	7.734	0.005	1
2921	A	57	TRP	HE3	7.381	0.005	1
2922	C	257	TRP	HE3	7.381	0.005	1
2923	A	57	TRP	HH2	6.689	0.010	1
2924	C	257	TRP	HH2	6.689	0.010	1
2925	A	57	TRP	HZ2	7.020	0.009	1
2926	C	257	TRP	HZ2	7.020	0.009	1
2927	A	57	TRP	HZ3	6.629	0.004	1
2928	C	257	TRP	HZ3	6.629	0.004	1
2929	A	57	TRP	C	178.829	0.1	1
2930	C	257	TRP	C	178.829	0.1	1
2931	A	57	TRP	CA	58.779	0.1	1
2932	C	257	TRP	CA	58.779	0.1	1
2933	A	57	TRP	CB	27.854	0.1	1
2934	C	257	TRP	CB	27.854	0.1	1
2935	A	57	TRP	CD1	128.680	0.1	1
2936	C	257	TRP	CD1	128.680	0.1	1
2937	A	57	TRP	CE3	121.176	0.1	1
2938	C	257	TRP	CE3	121.176	0.1	1
2939	A	57	TRP	CH2	124.023	0.1	1
2940	C	257	TRP	CH2	124.023	0.1	1
2941	A	57	TRP	CZ2	113.929	0.1	1
2942	C	257	TRP	CZ2	113.929	0.1	1
2943	A	57	TRP	CZ3	121.176	0.1	1
2944	C	257	TRP	CZ3	121.176	0.1	1
2945	A	57	TRP	N	113.503	0.1	1
2946	C	257	TRP	N	113.503	0.1	1
2947	A	58	ILE	H	6.449	0.003	1
2948	C	258	ILE	H	6.449	0.003	1
2949	A	58	ILE	HA	3.284	0.006	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2950	C	258	ILE	HA	3.284	0.006	1
2951	A	58	ILE	HB	1.770	0.005	1
2952	C	258	ILE	HB	1.770	0.005	1
2953	A	58	ILE	HD11	0.091	0.007	1
2954	C	258	ILE	HD11	0.091	0.007	1
2955	A	58	ILE	HD12	0.091	0.007	1
2956	C	258	ILE	HD12	0.091	0.007	1
2957	A	58	ILE	HD13	0.091	0.007	1
2958	C	258	ILE	HD13	0.091	0.007	1
2959	A	58	ILE	HG12	-0.417	0.004	2
2960	C	258	ILE	HG12	-0.417	0.004	2
2961	A	58	ILE	HG13	0.112	0.014	2
2962	C	258	ILE	HG13	0.112	0.014	2
2963	A	58	ILE	HG21	0.521	0.008	1
2964	C	258	ILE	HG21	0.521	0.008	1
2965	A	58	ILE	HG22	0.521	0.008	1
2966	C	258	ILE	HG22	0.521	0.008	1
2967	A	58	ILE	HG23	0.521	0.008	1
2968	C	258	ILE	HG23	0.521	0.008	1
2969	A	58	ILE	C	177.687	0.1	1
2970	C	258	ILE	C	177.687	0.1	1
2971	A	58	ILE	CA	64.177	0.1	1
2972	C	258	ILE	CA	64.177	0.1	1
2973	A	58	ILE	CB	35.710	0.1	1
2974	C	258	ILE	CB	35.710	0.1	1
2975	A	58	ILE	CD1	13.090	0.1	1
2976	C	258	ILE	CD1	13.090	0.1	1
2977	A	58	ILE	CG1	26.854	0.1	1
2978	C	258	ILE	CG1	26.854	0.1	1
2979	A	58	ILE	CG2	17.131	0.1	1
2980	C	258	ILE	CG2	17.131	0.1	1
2981	A	58	ILE	N	124.379	0.1	1
2982	C	258	ILE	N	124.379	0.1	1
2983	A	59	GLN	H	7.650	0.014	1
2984	C	259	GLN	H	7.650	0.014	1
2985	A	59	GLN	HA	3.747	0.020	1
2986	C	259	GLN	HA	3.747	0.020	1
2987	A	59	GLN	HB2	2.251	0.020	2
2988	C	259	GLN	HB2	2.251	0.020	2
2989	A	59	GLN	HB3	2.208	0.020	2
2990	C	259	GLN	HB3	2.208	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2991	A	59	GLN	HE21	7.984	0.003	2
2992	C	259	GLN	HE21	7.984	0.003	2
2993	A	59	GLN	HE22	7.144	0.020	2
2994	C	259	GLN	HE22	7.144	0.020	2
2995	A	59	GLN	HG2	2.393	0.020	2
2996	C	259	GLN	HG2	2.393	0.020	2
2997	A	59	GLN	HG3	2.393	0.020	2
2998	C	259	GLN	HG3	2.393	0.020	2
2999	A	59	GLN	C	178.361	0.1	1
3000	C	259	GLN	C	178.361	0.1	1
3001	A	59	GLN	CA	59.302	0.1	1
3002	C	259	GLN	CA	59.302	0.1	1
3003	A	59	GLN	CB	28.357	0.1	1
3004	C	259	GLN	CB	28.357	0.1	1
3005	A	59	GLN	CG	34.051	0.1	1
3006	C	259	GLN	CG	34.051	0.1	1
3007	A	59	GLN	N	118.966	0.1	1
3008	C	259	GLN	N	118.966	0.1	1
3009	A	59	GLN	NE2	115.755	0.001	1
3010	C	259	GLN	NE2	115.755	0.001	1
3011	A	60	GLU	H	8.075	0.005	1
3012	C	260	GLU	H	8.075	0.005	1
3013	A	60	GLU	HA	4.076	0.003	1
3014	C	260	GLU	HA	4.076	0.003	1
3015	A	60	GLU	HB2	2.250	0.012	2
3016	C	260	GLU	HB2	2.250	0.012	2
3017	A	60	GLU	HB3	2.101	0.007	2
3018	C	260	GLU	HB3	2.101	0.007	2
3019	A	60	GLU	HG2	2.546	0.003	2
3020	C	260	GLU	HG2	2.546	0.003	2
3021	A	60	GLU	HG3	2.270	0.009	2
3022	C	260	GLU	HG3	2.270	0.009	2
3023	A	60	GLU	C	179.019	0.1	1
3024	C	260	GLU	C	179.019	0.1	1
3025	A	60	GLU	CA	59.637	0.1	1
3026	C	260	GLU	CA	59.637	0.1	1
3027	A	60	GLU	CB	30.368	0.1	1
3028	C	260	GLU	CB	30.368	0.1	1
3029	A	60	GLU	CG	37.019	0.060	1
3030	C	260	GLU	CG	37.019	0.060	1
3031	A	60	GLU	N	117.105	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3032	C	260	GLU	N	117.105	0.1	1
3033	A	61	TYR	H	7.922	0.008	1
3034	C	261	TYR	H	7.922	0.008	1
3035	A	61	TYR	HA	4.237	0.020	1
3036	C	261	TYR	HA	4.237	0.020	1
3037	A	61	TYR	HB2	3.419	0.020	2
3038	C	261	TYR	HB2	3.419	0.020	2
3039	A	61	TYR	HB3	3.309	0.003	2
3040	C	261	TYR	HB3	3.309	0.003	2
3041	A	61	TYR	HD1	7.166	0.020	1
3042	C	261	TYR	HD1	7.166	0.020	1
3043	A	61	TYR	HD2	7.166	0.020	1
3044	C	261	TYR	HD2	7.166	0.020	1
3045	A	61	TYR	HE1	6.823	0.001	1
3046	C	261	TYR	HE1	6.823	0.001	1
3047	A	61	TYR	HE2	6.823	0.001	1
3048	C	261	TYR	HE2	6.823	0.001	1
3049	A	61	TYR	C	178.551	0.1	1
3050	C	261	TYR	C	178.551	0.1	1
3051	A	61	TYR	CA	61.206	0.1	1
3052	C	261	TYR	CA	61.206	0.1	1
3053	A	61	TYR	CB	39.669	0.1	1
3054	C	261	TYR	CB	39.669	0.1	1
3055	A	61	TYR	CD1	133.083	0.1	1
3056	C	261	TYR	CD1	133.083	0.1	1
3057	A	61	TYR	CE1	118.070	0.1	1
3058	C	261	TYR	CE1	118.070	0.1	1
3059	A	61	TYR	N	121.402	0.1	1
3060	C	261	TYR	N	121.402	0.1	1
3061	A	62	LEU	H	8.231	0.016	1
3062	C	262	LEU	H	8.231	0.016	1
3063	A	62	LEU	HA	3.967	0.020	1
3064	C	262	LEU	HA	3.967	0.020	1
3065	A	62	LEU	HB2	1.939	0.009	2
3066	C	262	LEU	HB2	1.939	0.009	2
3067	A	62	LEU	HB3	1.214	0.004	2
3068	C	262	LEU	HB3	1.214	0.004	2
3069	A	62	LEU	HD11	0.755	0.020	2
3070	C	262	LEU	HD11	0.755	0.020	2
3071	A	62	LEU	HD12	0.755	0.020	2
3072	C	262	LEU	HD12	0.755	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3073	A	62	LEU	HD13	0.755	0.020	2
3074	C	262	LEU	HD13	0.755	0.020	2
3075	A	62	LEU	HD21	0.696	0.020	2
3076	C	262	LEU	HD21	0.696	0.020	2
3077	A	62	LEU	HD22	0.696	0.020	2
3078	C	262	LEU	HD22	0.696	0.020	2
3079	A	62	LEU	HD23	0.696	0.020	2
3080	C	262	LEU	HD23	0.696	0.020	2
3081	A	62	LEU	HG	1.942	0.020	1
3082	C	262	LEU	HG	1.942	0.020	1
3083	A	62	LEU	C	179.458	0.1	1
3084	C	262	LEU	C	179.458	0.1	1
3085	A	62	LEU	CA	57.880	0.1	1
3086	C	262	LEU	CA	57.880	0.1	1
3087	A	62	LEU	CB	42.434	0.1	1
3088	C	262	LEU	CB	42.434	0.1	1
3089	A	62	LEU	CD1	23.192	0.1	1
3090	C	262	LEU	CD1	23.192	0.1	1
3091	A	62	LEU	CD2	26.727	0.1	1
3092	C	262	LEU	CD2	26.727	0.1	1
3093	A	62	LEU	CG	26.955	0.054	1
3094	C	262	LEU	CG	26.955	0.054	1
3095	A	62	LEU	N	116.209	0.1	1
3096	C	262	LEU	N	116.209	0.1	1
3097	A	63	GLU	H	8.467	0.020	1
3098	C	263	GLU	H	8.467	0.020	1
3099	A	63	GLU	HA	3.827	0.003	1
3100	C	263	GLU	HA	3.827	0.003	1
3101	A	63	GLU	HB2	2.241	0.007	2
3102	C	263	GLU	HB2	2.241	0.007	2
3103	A	63	GLU	HB3	2.075	0.020	2
3104	C	263	GLU	HB3	2.075	0.020	2
3105	A	63	GLU	HG2	2.473	0.020	2
3106	C	263	GLU	HG2	2.473	0.020	2
3107	A	63	GLU	HG3	2.254	0.008	2
3108	C	263	GLU	HG3	2.254	0.008	2
3109	A	63	GLU	C	179.166	0.1	1
3110	C	263	GLU	C	179.166	0.1	1
3111	A	63	GLU	CA	60.265	0.1	1
3112	C	263	GLU	CA	60.265	0.1	1
3113	A	63	GLU	CB	29.739	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3114	C	263	GLU	CB	29.739	0.1	1
3115	A	63	GLU	CG	37.207	0.1	1
3116	C	263	GLU	CG	37.207	0.1	1
3117	A	63	GLU	N	118.559	0.1	1
3118	C	263	GLU	N	118.559	0.1	1
3119	A	64	LYS	H	7.554	0.006	1
3120	C	264	LYS	H	7.554	0.006	1
3121	A	64	LYS	HA	4.215	0.007	1
3122	C	264	LYS	HA	4.215	0.007	1
3123	A	64	LYS	HB2	1.968	0.004	2
3124	C	264	LYS	HB2	1.968	0.004	2
3125	A	64	LYS	HB3	1.968	0.004	2
3126	C	264	LYS	HB3	1.968	0.004	2
3127	A	64	LYS	HD2	1.686	0.003	2
3128	C	264	LYS	HD2	1.686	0.003	2
3129	A	64	LYS	HD3	1.686	0.003	2
3130	C	264	LYS	HD3	1.686	0.003	2
3131	A	64	LYS	HE2	2.994	0.002	2
3132	C	264	LYS	HE2	2.994	0.002	2
3133	A	64	LYS	HE3	2.994	0.002	2
3134	C	264	LYS	HE3	2.994	0.002	2
3135	A	64	LYS	HG2	1.610	0.003	2
3136	C	264	LYS	HG2	1.610	0.003	2
3137	A	64	LYS	HG3	1.610	0.003	2
3138	C	264	LYS	HG3	1.610	0.003	2
3139	A	64	LYS	C	178.302	0.1	1
3140	C	264	LYS	C	178.302	0.1	1
3141	A	64	LYS	CA	58.481	0.062	1
3142	C	264	LYS	CA	58.481	0.062	1
3143	A	64	LYS	CB	32.505	0.1	1
3144	C	264	LYS	CB	32.505	0.1	1
3145	A	64	LYS	CD	29.379	0.1	1
3146	C	264	LYS	CD	29.379	0.1	1
3147	A	64	LYS	CE	42.579	0.108	1
3148	C	264	LYS	CE	42.579	0.108	1
3149	A	64	LYS	CG	25.465	0.1	1
3150	C	264	LYS	CG	25.465	0.1	1
3151	A	64	LYS	N	117.056	0.1	1
3152	C	264	LYS	N	117.056	0.1	1
3153	A	65	CYS	H	7.925	0.009	1
3154	C	265	CYS	H	7.925	0.009	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3155	A	65	CYS	HA	4.529	0.006	1
3156	C	265	CYS	HA	4.529	0.006	1
3157	A	65	CYS	HB2	3.084	0.004	2
3158	C	265	CYS	HB2	3.084	0.004	2
3159	A	65	CYS	HB3	3.015	0.010	2
3160	C	265	CYS	HB3	3.015	0.010	2
3161	A	65	CYS	C	174.775	0.1	1
3162	C	265	CYS	C	174.775	0.1	1
3163	A	65	CYS	CA	56.102	0.1	1
3164	C	265	CYS	CA	56.102	0.1	1
3165	A	65	CYS	CB	45.325	0.1	1
3166	C	265	CYS	CB	45.325	0.1	1
3167	A	65	CYS	N	115.236	0.1	1
3168	C	265	CYS	N	115.236	0.1	1
3169	A	66	LEU	H	7.541	0.020	1
3170	C	266	LEU	H	7.541	0.020	1
3171	A	66	LEU	HA	4.520	0.020	1
3172	C	266	LEU	HA	4.520	0.020	1
3173	A	66	LEU	HB2	1.725	0.013	2
3174	C	266	LEU	HB2	1.725	0.013	2
3175	A	66	LEU	HB3	1.584	0.020	2
3176	C	266	LEU	HB3	1.584	0.020	2
3177	A	66	LEU	HD11	0.873	0.020	2
3178	C	266	LEU	HD11	0.873	0.020	2
3179	A	66	LEU	HD12	0.873	0.020	2
3180	C	266	LEU	HD12	0.873	0.020	2
3181	A	66	LEU	HD13	0.873	0.020	2
3182	C	266	LEU	HD13	0.873	0.020	2
3183	A	66	LEU	HD21	0.868	0.003	2
3184	C	266	LEU	HD21	0.868	0.003	2
3185	A	66	LEU	HD22	0.868	0.003	2
3186	C	266	LEU	HD22	0.868	0.003	2
3187	A	66	LEU	HD23	0.868	0.003	2
3188	C	266	LEU	HD23	0.868	0.003	2
3189	A	66	LEU	HG	1.700	0.020	1
3190	C	266	LEU	HG	1.700	0.020	1
3191	A	66	LEU	C	176.765	0.1	1
3192	C	266	LEU	C	176.765	0.1	1
3193	A	66	LEU	CA	55.202	0.1	1
3194	C	266	LEU	CA	55.202	0.1	1
3195	A	66	LEU	CB	43.314	0.1	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3196	C	266	LEU	CB	43.314	0.1	1
3197	A	66	LEU	CD1	26.475	0.1	1
3198	C	266	LEU	CD1	26.475	0.1	1
3199	A	66	LEU	CD2	23.823	0.1	1
3200	C	266	LEU	CD2	23.823	0.1	1
3201	A	66	LEU	CG	26.601	0.1	1
3202	C	266	LEU	CG	26.601	0.1	1
3203	A	66	LEU	N	121.130	0.1	1
3204	C	266	LEU	N	121.130	0.1	1
3205	A	67	ASN	H	8.306	0.005	1
3206	C	267	ASN	H	8.306	0.005	1
3207	A	67	ASN	HA	4.639	0.020	1
3208	C	267	ASN	HA	4.639	0.020	1
3209	A	67	ASN	HB2	2.846	0.020	2
3210	C	267	ASN	HB2	2.846	0.020	2
3211	A	67	ASN	HB3	2.604	0.020	2
3212	C	267	ASN	HB3	2.604	0.020	2
3213	A	67	ASN	HD21	7.595	0.006	2
3214	C	267	ASN	HD21	7.595	0.006	2
3215	A	67	ASN	HD22	6.857	0.003	2
3216	C	267	ASN	HD22	6.857	0.003	2
3217	A	67	ASN	C	174.189	0.1	1
3218	C	267	ASN	C	174.189	0.1	1
3219	A	67	ASN	CA	53.654	0.1	1
3220	C	267	ASN	CA	53.654	0.1	1
3221	A	67	ASN	CB	38.978	0.1	1
3222	C	267	ASN	CB	38.978	0.1	1
3223	A	67	ASN	N	120.313	0.095	1
3224	C	267	ASN	N	120.313	0.095	1
3225	A	67	ASN	ND2	112.192	0.1	1
3226	C	267	ASN	ND2	112.192	0.1	1
3227	A	68	LYS	H	7.913	0.008	1
3228	C	268	LYS	H	7.913	0.008	1
3229	A	68	LYS	HA	4.667	0.020	1
3230	C	268	LYS	HA	4.667	0.020	1
3231	A	68	LYS	HB2	1.830	0.020	2
3232	C	268	LYS	HB2	1.830	0.020	2
3233	A	68	LYS	HD2	1.411	0.020	2
3234	C	268	LYS	HD2	1.411	0.020	2
3235	A	68	LYS	HG2	1.713	0.020	2
3236	C	268	LYS	HG2	1.713	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3237	A	68	LYS	N	127.077	0.1	1
3238	C	268	LYS	N	127.077	0.1	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	122	-0.18 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	122	-0.32 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}'$	116	-0.09 ± 0.23	None needed (< 0.5 ppm)
^{15}N	120	0.10 ± 0.20	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 84%, i.e. 1251 atoms were assigned a chemical shift out of a possible 1484. 20 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	509/537 (95%)	206/214 (96%)	200/218 (92%)	103/105 (98%)
Sidechain	670/839 (80%)	418/496 (84%)	242/292 (83%)	10/51 (20%)
Aromatic	72/108 (67%)	42/56 (75%)	30/42 (71%)	0/10 (0%)
Overall	1251/1484 (84%)	666/766 (87%)	472/552 (86%)	113/166 (68%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 1474 atoms were assigned a chemical shift out of a possible 1834. 22 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	602/664 (91%)	244/264 (92%)	238/272 (88%)	120/128 (94%)
Sidechain	788/1046 (75%)	496/622 (80%)	280/358 (78%)	12/66 (18%)
Aromatic	84/124 (68%)	50/64 (78%)	34/50 (68%)	0/10 (0%)
Overall	1474/1834 (80%)	790/950 (83%)	552/680 (81%)	132/204 (65%)

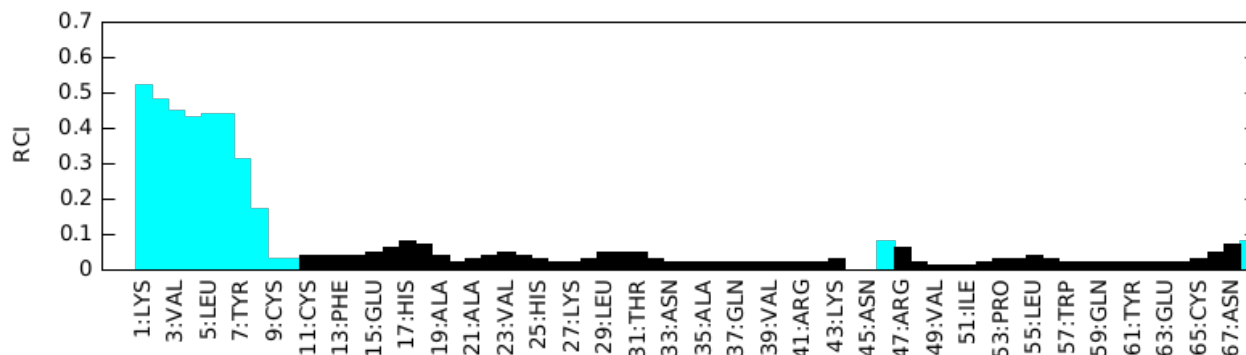
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The images below report *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain C:

